

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

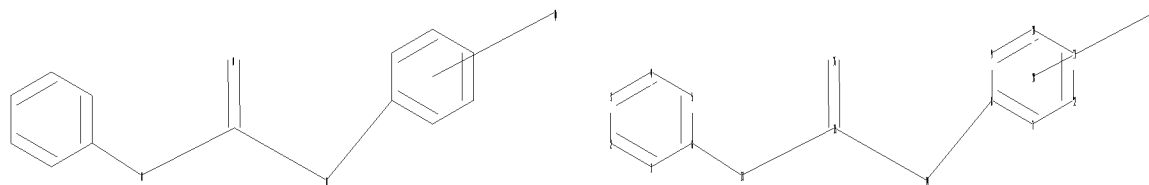
LOGINID:SSPTACDR1614

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	3	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	4	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	5	APR 28	IMSRESEARCH reloaded with enhancements
NEWS	6	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS	7	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	8	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	9	JUN 06	KOREAPAT updated with 41,000 documents
NEWS	10	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS	11	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS	12	JUN 25	CA/CAPLUS and USPAT databases updated with IPC reclassification data
NEWS	13	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS	14	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS	15	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS	16	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS	17	JUL 28	CA/CAPLUS patent coverage enhanced
NEWS	18	JUL 28	EPFULL enhanced with additional legal status information from the epline Register
NEWS	19	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS	20	JUL 28	STN Viewer performance improved
NEWS	21	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS	22	AUG 13	CA/CAPLUS enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS	23	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	24	AUG 15	CAPLUS currency for Korean patents enhanced
NEWS	25	AUG 25	CA/CAPLUS, CASREACT, and IFI and USPAT databases enhanced for more flexible patent number searching
NEWS	26	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS	27	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS	28	SEP 25	CA/CAPLUS current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances



```

chain nodes :
13 14 15 16 17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
6-13 8-14 13-15 14-15 15-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
6-13 8-14 13-15 14-15 15-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

```

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom
Generic attributes :
17:
Saturation           : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System   : Polycyclic

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Element Count :
Node 17: Limited
  N,N4
  C,C5

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L1 STRUCTURE UPLOADED

```

=> s l1 sss sam
SAMPLE SEARCH INITIATED 10:19:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9200 TO ITERATE

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21.7% PROCESSED      2000 ITERATIONS                      6 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

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FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   178251 TO 189749
PROJECTED ANSWERS:      237 TO 867

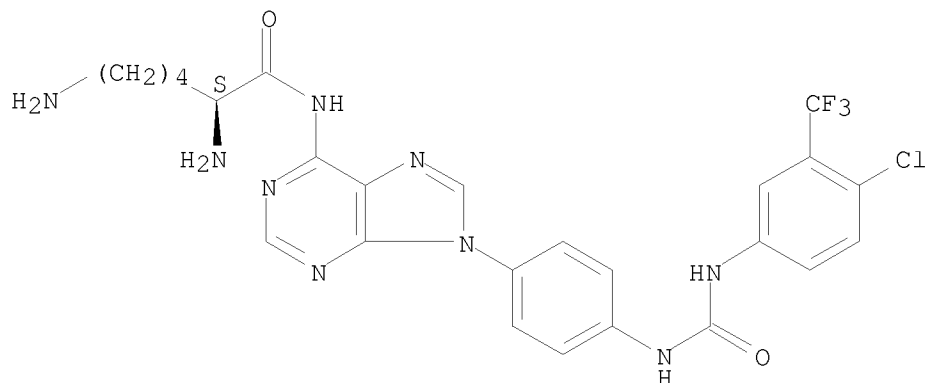
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L2 6 SEA SSS SAM L1

=> d scan

L2 6 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Hexanamide, 2,6-diamino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, (2S)-
MF C25 H25 Cl F3 N9 O2
CI COM

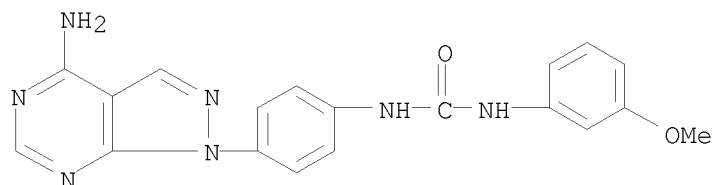
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 6 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Urea, N-[4-(4-amino-1H-pyrazolo[3,4-d]pyrimidin-1-yl)phenyl]-N'-(3-methoxyphenyl)-
MF C19 H17 N7 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s ll sss full

FULL SEARCH INITIATED 10:20:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 184298 TO ITERATE

100.0% PROCESSED 184298 ITERATIONS
SEARCH TIME: 00.00.05

481 ANSWERS

L3 481 SEA SSS FUL L1

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.82

179.03

FILE 'REGISTRY' ENTERED AT 10:20:28 ON 29 SEP 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 SEP 2008 HIGHEST RN 1053621-88-7

DICTIONARY FILE UPDATES: 26 SEP 2008 HIGHEST RN 1053621-88-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.46

179.49

FILE 'CAPLUS' ENTERED AT 10:20:41 ON 29 SEP 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 29 Sep 2008 VOL 149 ISS 14

FILE LAST UPDATED: 28 Sep 2008 (20080928/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> s 13

L4 27 L3

=> d ibib abs hitstr 27

L4 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1963:436076 CAPLUS
DOCUMENT NUMBER: 59:36076
ORIGINAL REFERENCE NO.: 59:6555a-f
TITLE: Pyridotriazole brighteners
INVENTOR(S): Buell, Bennett G.; Long, Robert S.
PATENT ASSIGNEE(S): American Cyanamid Co.
SOURCE: 11 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

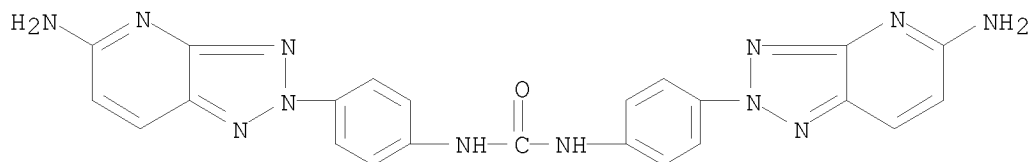
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3049438		19620814	US 1958-771175	19581103
PRIORITY APPLN. INFO.:			US	19581103

GI For diagram(s), see printed CA Issue.

AB Compds. of the structures I or II, in which Y is H, alkyl, halogen, or carboxyl, n is 1 or 2, R is the residue of a diazotizable amine, R' is Me or Et, and X- is halide or other anion, exhibit phosphorescence and fluorescence, and are stable to the conditions of textile manufacture. By proper selection of substituents, they can be used to brighten a wide range of synthetic and natural fibers. Thus, a mixture of 2,6-diamino-3-(phenylazo)pyridine 27.9, EtOH 450, H₂O 70, and concentrated aqueous NH₃ 180 parts was refluxed with stirring, and a hot solution of CuSO₄ 170 in H₂O 500 and concentrated aqueous NH₃ 300 parts added. After several hrs., CuSO₄ 25 in H₂O 125 and concentrated aqueous NH₃ 45 parts was added and heating continued to complete reaction. The product was cooled, filtered, washed with dilute aqueous NH₃ and H₂O, dissolved in H₂O 400, EtOH 450, and concentrated HCl 150 parts, the solution treated with a decolorizing agent, filtered, and 55 parts concentrated HCl added. The precipitated hydrochloride (III) was filtered and washed with EtOH. A 1:1000 solution of III in HCONMe₂ was diluted with H₂O containing a dispersing agent to 0.005%, and this solution 50 added to H₂O 98.5 and AcOH 1.5 parts. Orlon fabric was boiled in the solution 30 min., removed, washed, and dried. It was much whiter and brighter than untreated fabric. The following I were similarly prepared (R, Y, and n given): 3,4-NaO₃S(PhCH:CH)C₆H₃, H, 1; 4-NaO₃SC₆H₄, H, 1; p-PhC₆H₄, H, 1; Ph, 6-Br, 1; p-PhC₆H₄, 7-Me, 1; p-H₂NC₆H₄, H, 1; p-(p-MeOC₆H₄CONH)C₆H₄, H, 1; p-(5-sulfo-2H-naphtho[1,2-d]triazol-2-yl)phenyl (Na salt), H, 1; p-biphenylene, H, 2; vinylenebis(3-sulfo-p-phenylene) (Na salt), H, 2; 2,7-dihydro-4-methyl-7-(4-sulfophenyl)-2-benzo[1,2-d:3,4-d']bistriazolyl, H, 1; Ph, 7-CO₂H, 1; p-ClC₆H₄, H, 1; 3,4-Me₂C₆H₃, H, 1; 2-naphthyl, H, 1; p-(PhCH:CH)C₆H₄, H, 1; 3,4-NC(PhCH:CH)C₆H₃, H, 1; 3,4-NC(o-HO₃SC₆H₄CH:CH)C₆H₃, H, 1; 4-(4-benzamido-2-sulfostyryl)-3-sulfophenyl, H, 1; p-(6-methyl-2-benzothiazolyl)phenyl, H, 1; 4-(2-benzoxazolyl)phenyl, H, 1; 4-(2-benzimidazolyl)phenyl, H, 1; 5-benzothiazolyl, H, 1;

2-phenyl-6-benzoxazolyl, H, 1; 2-methyl-5-benzimidazolyl, H, 1;
 3-sulfo-p-biphenylylene, H, 2; vinylenedi-p-phenylene, H, 2;
 iminodi-p-phenylene, H, 2; 5,5-dioxo-3,6-dibenzothiophenediyl, H, 2;
 ureylenedi-p-phenylene, H, 2; p-(7-sulfo-2H-naphtho[1,2-d]triazol-2-
 yl)phenyl, H, 1; m-BrC6H4, H, 1; 4-pyridyl, H, 1; 5-pyrimidinyl, H, 1. A
 mixture of I (R = Ph, Y = H, n = 1) 1, MeOH 40, and MeI 44 parts was
 refluxed until the reaction was completed, evaporated to dryness, and the
 residue recrystd. from MeOH-Et2O to give II (R = Ph, R' = Me, X- =
 iodide). Similarly prepared were II (R, R', X- given): Ph, Et, EtOSO3-; Ph,
 Me, p-MeC6H4SO3-; p-PhC6H4, Me, iodide.

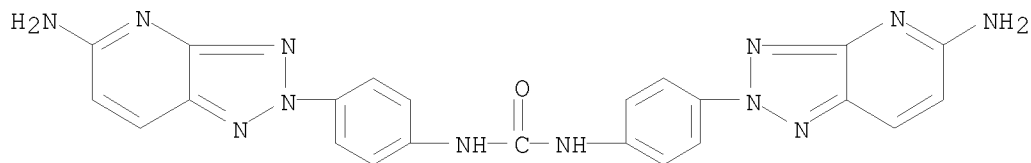
IT 15785-02-1P, Carbanilide, 4,4'-bis(5-amino-2H-v-triazolo[4,5-b]-
 pyridin-2-yl)-
 RL: PREP (Preparation)
 (preparation of)
 RN 15785-02-1 CAPLUS
 CN Carbanilide, 4,4'-bis(5-amino-2H-v-triazolo[4,5-b]pyridin-2-yl)- (7CI,
 8CI) (CA INDEX NAME)



=> d ibib abs hitstr 26

L4 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1967:19830 CAPLUS
 DOCUMENT NUMBER: 66:19830
 ORIGINAL REFERENCE NO.: 66:3843a,3846a
 TITLE: Pyridotriazole brighteners
 INVENTOR(S): Buell, Bennett G.; Long, Robert S.
 PATENT ASSIGNEE(S): American Cyanamid Co.
 SOURCE: U.S., 11 pp. Division of U.S. 3222371
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

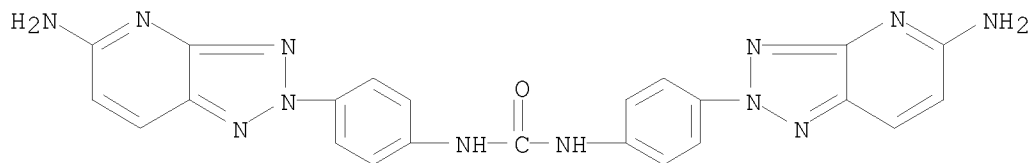
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	US 260295		19660913	US	19640825
AB	Division of U.S. 3,222,371 (CA 64, 6799h). The disclosure is the same but the claims are different.				
IT	15785-02-1P RL: IMF (Industrial manufacture); PREP (Preparation) (preparation of)				
RN	15785-02-1 CAPLUS				
CN	Carbanilide, 4,4'-bis(5-amino-2H-v-triazolo[4,5-b]pyridin-2-yl)- (7CI, 8CI) (CA INDEX NAME)				



=> d ibib abs hitstr 25

L4 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1967:19831 CAPLUS
 DOCUMENT NUMBER: 66:19831
 ORIGINAL REFERENCE NO.: 66:3843a,3846a
 TITLE: Pyridotriazole brighteners
 INVENTOR(S): Buell, Bennett G.; Long, Robert S.
 PATENT ASSIGNEE(S): American Cyanamid Co.
 SOURCE: U.S., 11 pp. Division of U.S. 3222371
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	US 3272830		19660913	US 1964-392047	19640825
AB	Division of U.S. 3,222,371 (CA 64, 6799h). The disclosure is the same but the claims are different.				
IT	15785-02-1P				
	RL: IMF (Industrial manufacture); PREP (Preparation) (preparation of)				
RN	15785-02-1	CAPLUS			
CN	Carbanilide, 4,4'-bis(5-amino-2H-v-triazolo[4,5-b]pyridin-2-yl)- (7CI, 8CI) (CA INDEX NAME)				

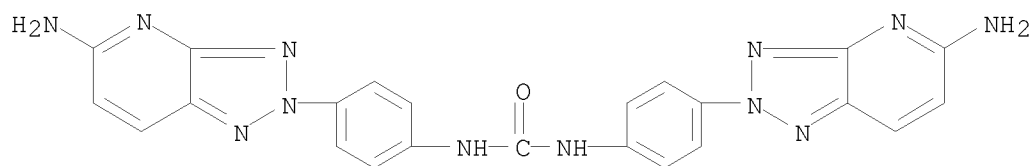


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L4 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1967:19832 CAPLUS
 DOCUMENT NUMBER: 66:19832
 ORIGINAL REFERENCE NO.: 66:3843a,3846a
 TITLE: Pyridotriazole brighteners
 INVENTOR(S): Buell, Bennett G.; Long, Robert S.
 PATENT ASSIGNEE(S): American Cyanamid Co.
 SOURCE: U.S., 11 pp. Division of U.S. 3222371
 CODEN: USXXAM
 DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
	US 3272831		19660913	US 1964-392048	19640825
AB	Division of U.S. 3,222,371 (CA 64, 6799h). The disclosure is the same but the claims are different.				
IT	15785-02-1P				
	RL: IMF (Industrial manufacture); PREP (Preparation) (preparation of)				
RN	15785-02-1	CAPLUS			
CN	Carbanilide, 4,4'-bis(5-amino-2H-v-triazolo[4,5-b]pyridin-2-yl)- (7CI, 8CI) (CA INDEX NAME)				



=> d ibib abs hitstr 23

L4 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:433164 CAPLUS

DOCUMENT NUMBER: 69:33164

ORIGINAL REFERENCE NO.: 69:6175a,6178a

TITLE: Irreversible enzyme inhibitors. CXXIII. Candidate irreversible inhibitors of guanine deaminase and xanthine oxidase derived from 9-phenylguanine substituted with a terminal sulfonyl fluoride

AUTHOR(S): Baker, B. R.; Wood, William F.

CORPORATE SOURCE: Univ. of California, Santa Barbara, CA, USA

SOURCE: Journal of Medicinal Chemistry (1968), 11(4), 650-2
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 9-[p-(p-Fluorosulfonylbenzamido)phenyl]guanine (I) at 0.7×10^{-6} M was an excellent active-site-directed irreversible inhibitor of xanthine oxidase, causing 85% inactivation in 1 min. at 37° and 97% in 24 min.; in contrast, I fails to inactivate guanine deaminase at 21×10^{-6} M. When the fluorosulfonylbenzamido moiety was moved to the meta position, better reversible inhibitors emerged, but no irreversible inhibition of either xanthine oxidase or guanine deaminase occurred.

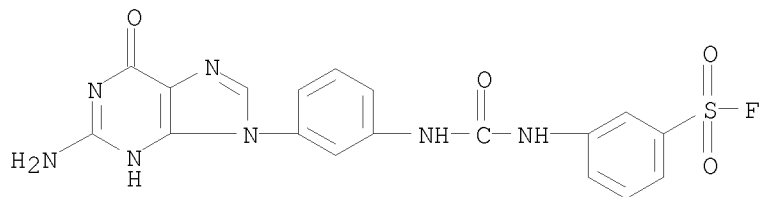
IT 21318-99-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of and inhibition of guanine deaminase and xanthine oxidase by)

RN 21318-99-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



=> d ibib abs hitstr 22

L4 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:433166 CAPLUS

DOCUMENT NUMBER: 69:33166

ORIGINAL REFERENCE NO.: 69:6175a,6178a

TITLE: Irreversible enzyme inhibitors. CXXV. Active site-directed irreversible inhibitors of xanthine oxidase derived from arylpurines and pyrazolo[3,4-d]pyrimidines bearing a terminal sulfonyl fluoride

AUTHOR(S): Baker, B. R.; Kozma, Janos A.

CORPORATE SOURCE: Univ. of California, Santa Barbara, CA, USA

SOURCE: Journal of Medicinal Chemistry (1968), 11(4), 656-61
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

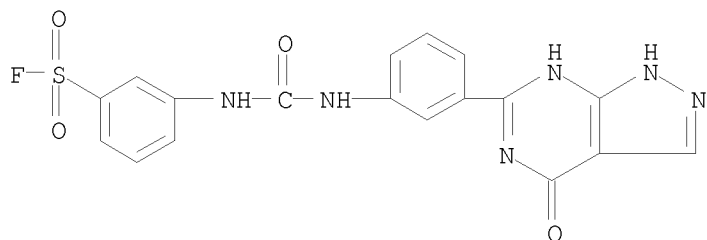
AB 4-Hydroxy-6-phenylpyrazolo [3,4-d]pyrimidines with m-fluorosulfonylbenzamido (I) or p-fluorosulfonylbenzamido (II) groups on the meta position are active-sitedirected irreversible inhibitors of xanthine oxidase; in contrast, the m-fluorosulfonylbenzamido substituent on the para position does not give an irreversible inhibitor. Replacement of the 4-hydroxy group of I or II by amino gives no loss of reversible inhibition, but irreversible inhibition is eradicated. Similarly, these fluorosulfonylbenzamido groups in the meta or para position of 8-phenyladenine afford better reversible inhibitors, but irreversible inhibition is again lost. The 7 types of active-sitedirected irreversible inhibitors of xanthine oxidase found to date are compared in efficiency.

IT 21319-18-6P 21412-54-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and xanthine oxidase inhibition by)

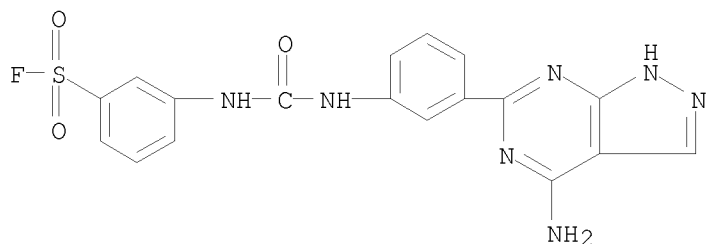
RN 21319-18-6 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



RN 21412-54-4 CAPLUS

CN Metanilyl fluoride, N-[[[m-(4-amino-1H-pyrazolo[3,4-d]pyrimidin-6-yl)phenyl]carbonyl]- (8CI) (CA INDEX NAME)



=> d ibib abs hitstr 21

L4 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:96759 CAPLUS

DOCUMENT NUMBER: 70:96759

ORIGINAL REFERENCE NO.: 70:18085a,18088a

TITLE: Irreversible enzyme inhibitors. CXLVI.
Active-site-directed irreversible inhibitors of
xanthine oxidase derived from 9-
(acylamidophenyl)guanines substituted with a terminal
phenylenesulfonyl fluoride

AUTHOR(S): Baker, Bernard Randall; Wood, William F.

CORPORATE SOURCE: Univ. of California, Santa Barbara, CA, USA

SOURCE: Journal of Medicinal Chemistry (1969), 12(2), 211-14
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

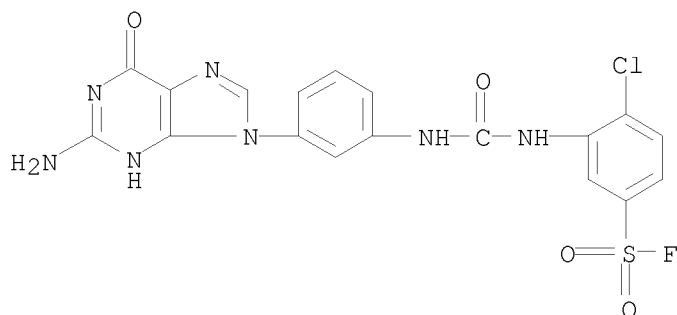
AB Twenty candidate active-site-directed irreversible inhibitors of xanthine oxidase have been synthesized and evaluated. These were derived from m- or p-amino-9-phenylguanine attached to benzenesulfonyl fluoride by a sulfonamide, carboxamide, or urea bridge. Three excellent irreversible inhibitors emerged that at a concentration of 10^{-6} to 10^{-7} M gave total inactivation of xanthine oxidase with a half-life of 1 min. or less; these were 9-phenylguanines substituted by a p-(p-fluorosulfonylbenzamido), p-(m-fluorosulfonylbenzamido), or m-(p-fluorosulfonylbenzenesulfonamido) moiety.

IT 20566-66-9P 21864-31-3P 21864-34-6P
21864-35-7P 21864-36-8P 21864-38-0P
21952-25-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

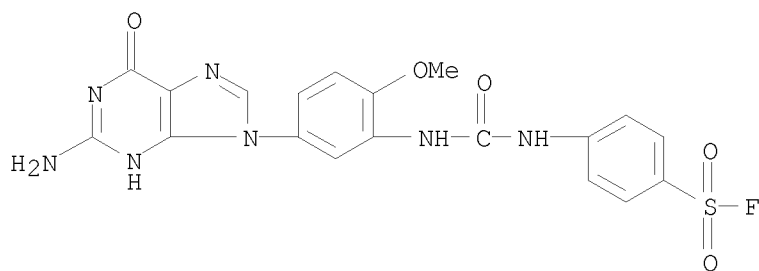
RN 20566-66-9 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)



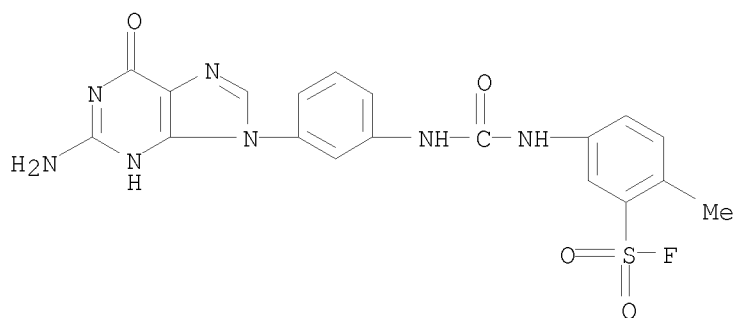
RN 21864-31-3 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



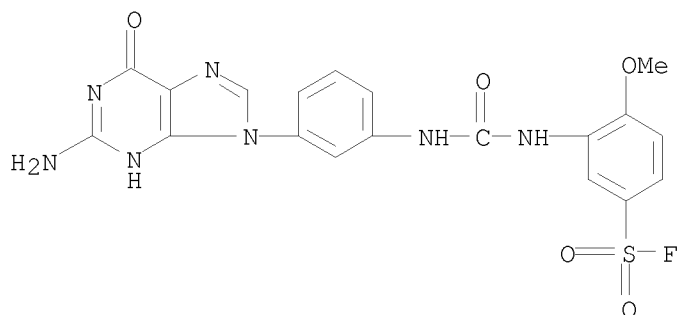
RN 21864-34-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)



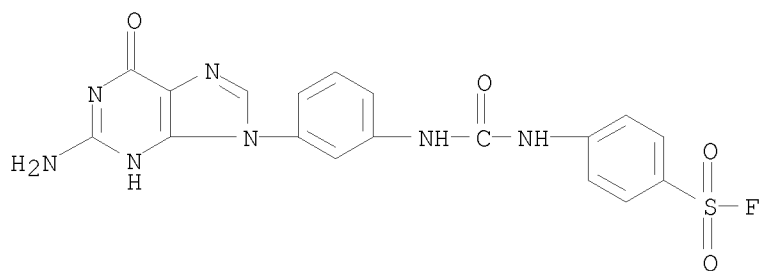
RN 21864-35-7 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)



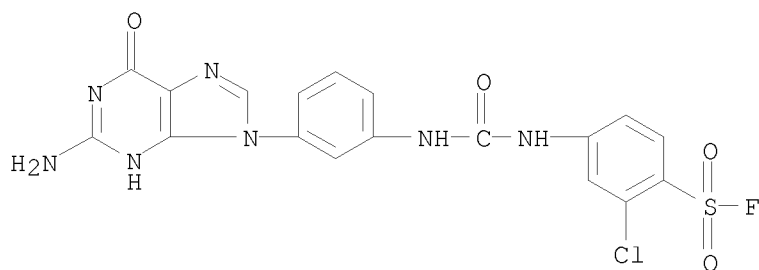
RN 21864-36-8 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



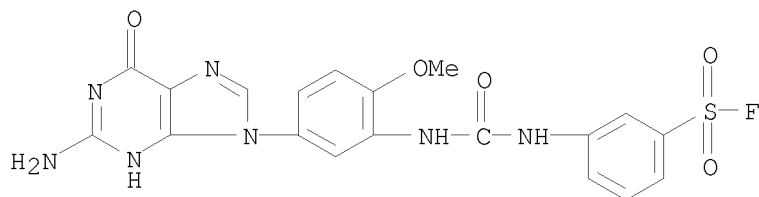
RN 21864-38-0 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



RN 21952-25-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



=> d ibib abs hitstr 20

L4 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:103224 CAPLUS

DOCUMENT NUMBER: 70:103224

ORIGINAL REFERENCE NO.: 70:19261a,19264a

TITLE: Irreversible enzyme inhibitors. CXLVIII.
Active-site-directed irreversible inhibitors of
guanine deaminase derived from p-phenylguanine bearing
a terminal phenylenesulfonyl fluoride

AUTHOR(S): Baker, Bernard Randall; Wood, William F.

CORPORATE SOURCE: Univ. of California, Santa Barbara, CA, USA

SOURCE: Journal of Medicinal Chemistry (1969), 12(2), 216-20

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Thirty-eight candidate irreversible inhibitors of guanine deaminase
derived from 9-phenylguanine with a terminal sulfonyl fluoride bridged to
the meta or para position of the phenyl moiety by an amide or ether
linkage were evaluated with the enzyme from Walker 256 rat tumor. Three
of the compds. (I-III) were excellent irreversible inhibitors of this
enzyme, but also showed no isozyme specificity since these could also
inactivate the rat liver enzyme. Of the 13 compds. showing moderate
irreversible inhibition of the Walker 256 enzyme, 4 (IV-VII) showed
isozyme specificity with no inactivation of the rat liver enzyme.

IT 20566-66-9 21318-99-0 21864-31-3

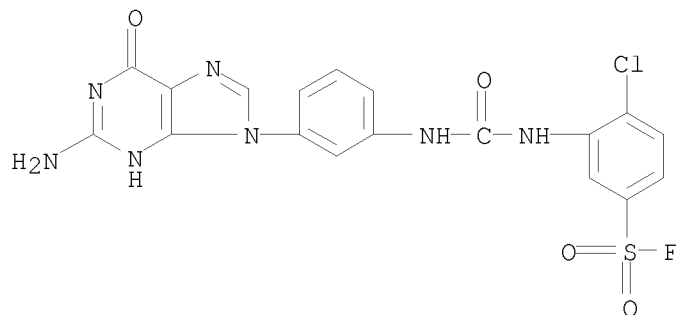
21864-34-6 21864-35-7 21864-36-8

21864-38-0 21952-25-0

RL: BIOL (Biological study)
(guanine deaminase inhibition by)

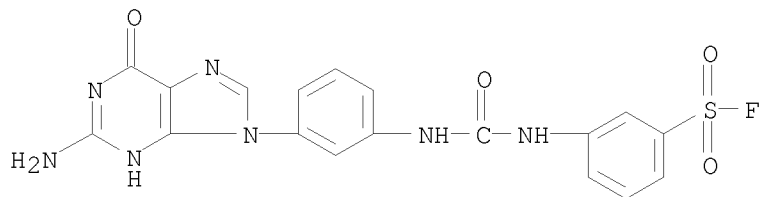
RN 20566-66-9 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)



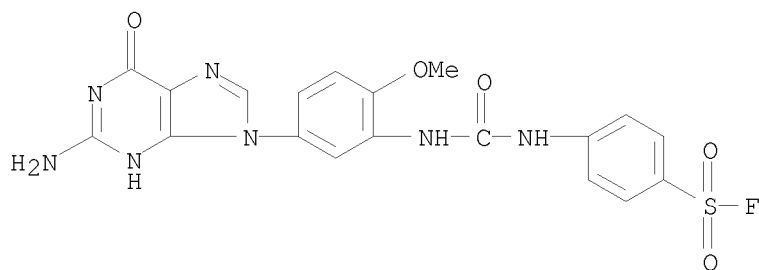
RN 21318-99-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



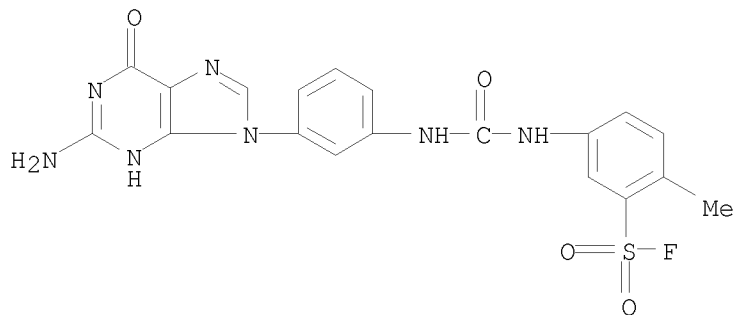
RN 21864-31-3 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



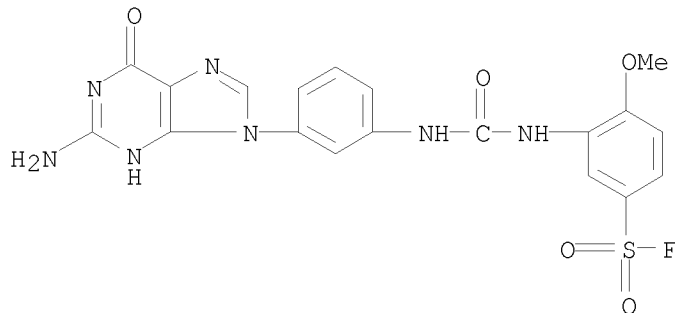
RN 21864-34-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)

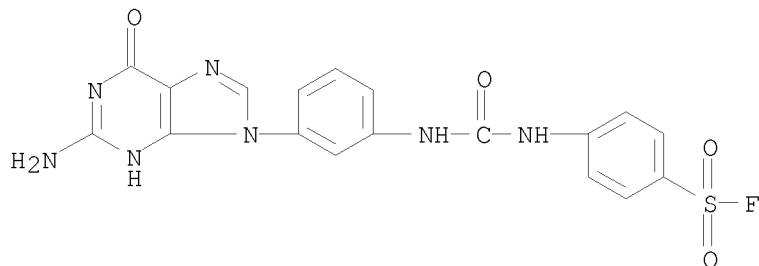


RN 21864-35-7 CAPLUS

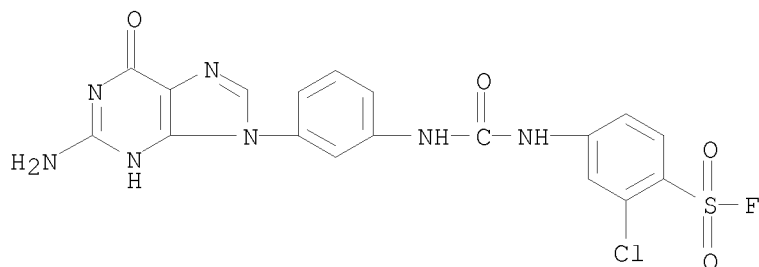
CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)



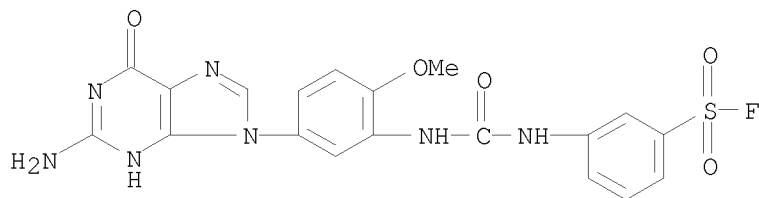
RN 21864-36-8 CAPLUS
 CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



RN 21864-38-0 CAPLUS
 CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



RN 21952-25-0 CAPLUS
 CN Benzenesulfonyl fluoride, 3-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



=> d ibib abs hitstr 19

L4 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1971:529761 CAPLUS
 DOCUMENT NUMBER: 75:129761
 ORIGINAL REFERENCE NO.: 75:20487a,20490a
 TITLE: Irreversible enzyme inhibitors. 185.
 Active-site-directed irreversible inhibitors of
 guanine deaminase derived from 9-phenylguanine bearing
 a terminal sulfonyl fluoride. 2
 AUTHOR(S): Baker, B. R.; Siebeneick, Hans U.

CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA, USA
SOURCE: Journal of Medicinal Chemistry (1971), 14(9), 802-5
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

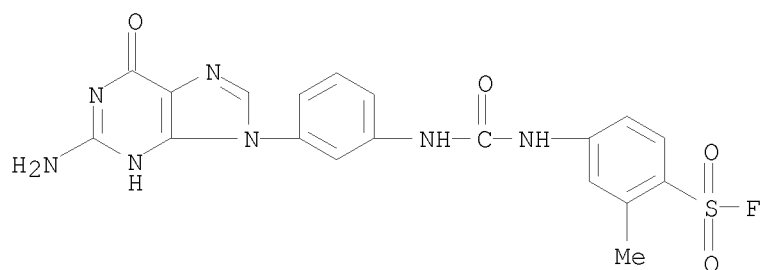
AB Eleven derivs. of 9-phenylguanine bridged from its meta position and 11 derivs. of 9-(p-ethoxyphenyl)guanine bridged from its terminal Me group by carboxamide or ureido bridges to substituted benzenesulfonyl fluorides were synthesized and investigated as irreversible inhibitors of Walker 256 rat tumor guanine deaminase. Four of these compds., 9-[3-(4-chloro-3-fluorosulfonylbenzamido)phenyl]guanine (I), 9-[3-(2,4-dichloro-3-fluorosulfonylbenzamido)phenyl]guanine (II), 9-[3-(3-chloro-4-fluorosulfonylbenzamido)phenyl]guanine (III), and 9-[3-(4-fluorosulfonyl-3-methylbenzamido)phenyl]guanine (IV), gave essentially complete inactivation of the tumor enzyme, but failed to show tissue specificity, since rat liver guanine deaminase was also inactivated by these compds. The 2 acetylamido series were prepared by acylation of 9-(m-aminophenyl)guanine or 9-(p-aminoethoxyphenyl)guanine with the appropriate acid chloride. The 2 phenylureido series were synthesized by condensation of the 2 amines with appropriate O-(p-nitrophenyl)-N-arylcarbamate.

IT 33873-39-1P 33873-40-4P 33873-41-5P
33873-42-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

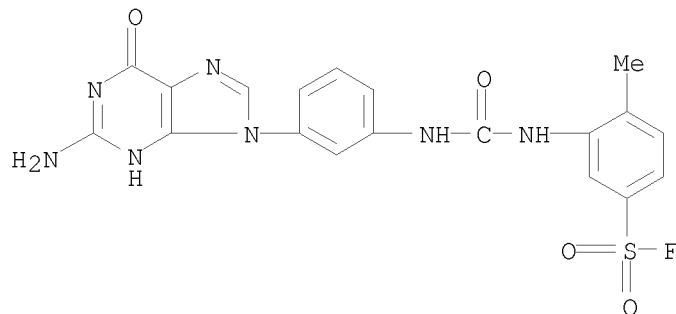
RN 33873-39-1 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)



RN 33873-40-4 CAPLUS

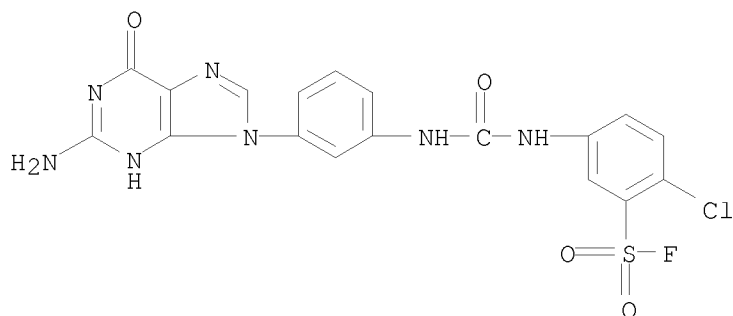
CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methyl- (CA INDEX NAME)



RN 33873-41-5 CAPLUS

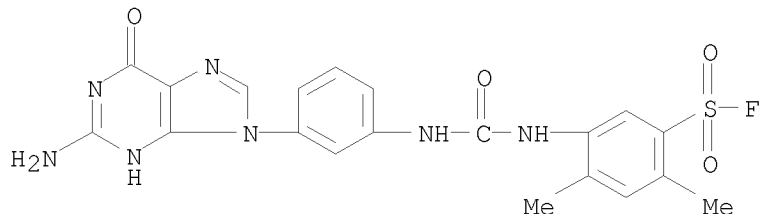
CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-

yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



RN 33873-42-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2,4-dimethyl- (CA INDEX NAME)



=> d ibib abs hitstr 18

L4 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1976:38576 CAPLUS

DOCUMENT NUMBER: 84:38576

ORIGINAL REFERENCE NO.: 84:6271a,6274a

TITLE: Correlation analysis of Baker's studies on enzyme inhibition. 1. Guanine deaminase, xanthine oxidase, dihydrofolate reductase, and complement

AUTHOR(S): Silipo, Carlo; Hansch, Corwin

CORPORATE SOURCE: Dep. Chem., Pomona Coll., Claremont, CA, USA

SOURCE: Journal of Medicinal Chemistry (1976), 19(1), 62-71

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two correlation equations were developed relating inhibitory activity of guanine deaminase [9033-16-3] and xanthine oxidase [9002-17-9] inhibitors to their chemical structure. These equations were based on data obtained by B.R. Baker (1967) using .apprx.90 inhibitors of these 2 enzyme systems. The importance of indicator variables in correlation anal. of enzymes for drug development was discussed.

IT 20566-66-9 21318-99-0 21864-31-3

21864-34-6 21864-35-7 21864-36-8

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33873-40-4 33873-41-5 33873-42-6

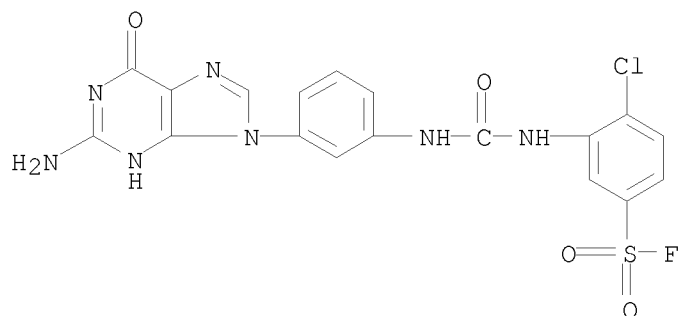
RL: BIOL (Biological study)

(enzyme inhibition by, correlation anal. of)

RN 20566-66-9 CAPLUS

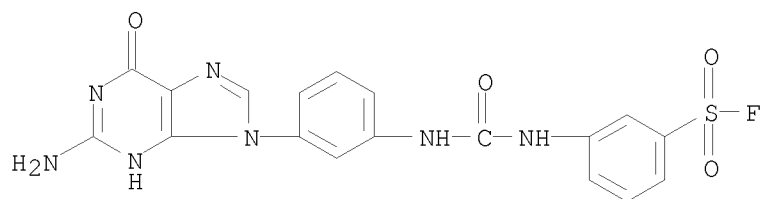
CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-

yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)



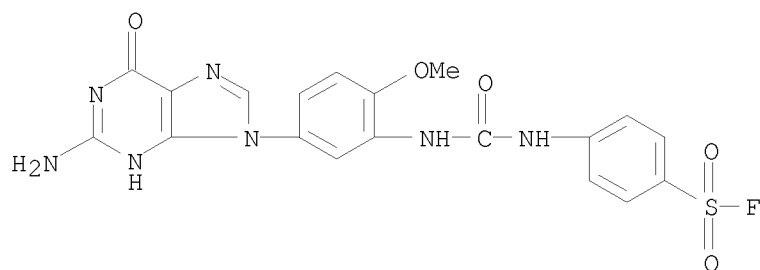
RN 21318-99-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



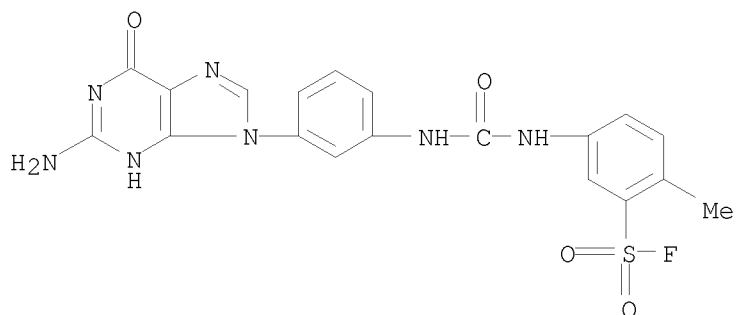
RN 21864-31-3 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



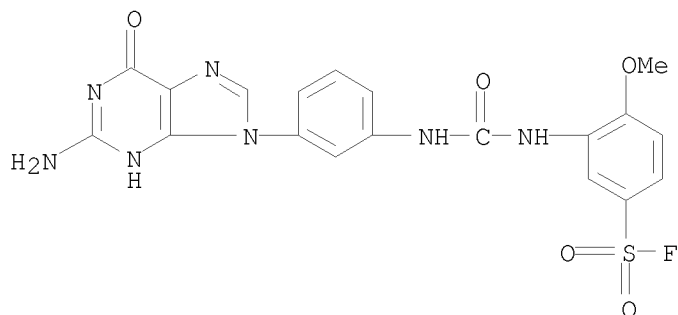
RN 21864-34-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)



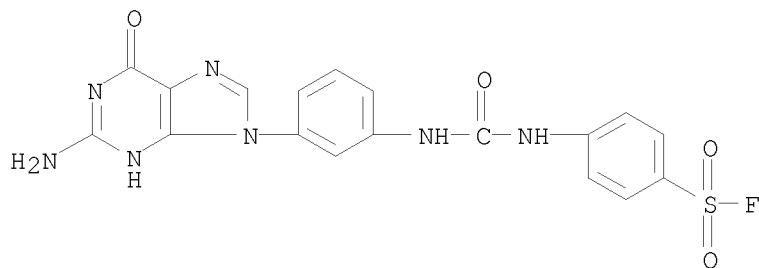
RN 21864-35-7 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)



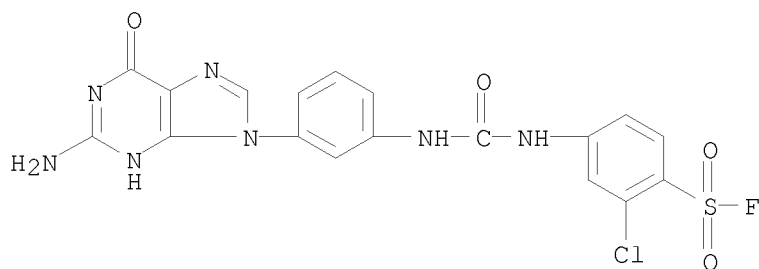
RN 21864-36-8 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



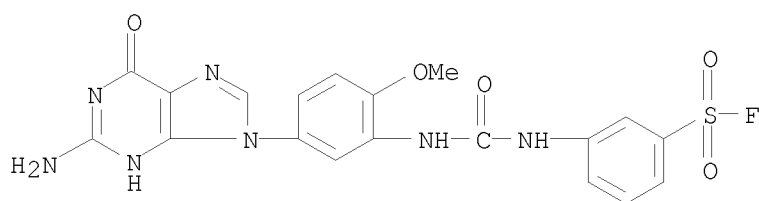
RN 21864-38-0 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



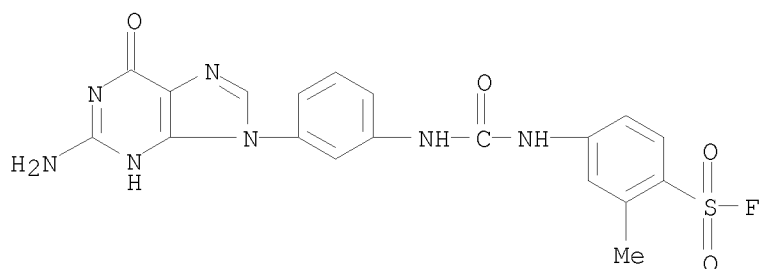
RN 21952-25-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



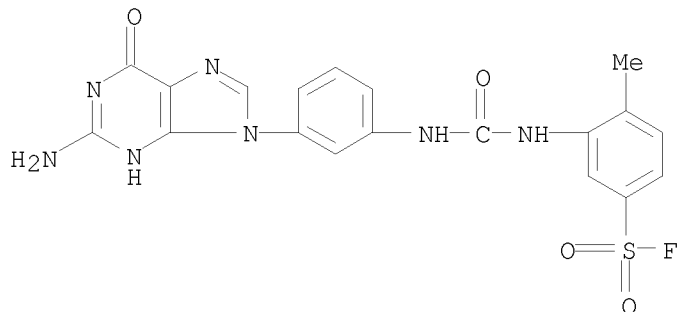
RN 33873-39-1 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)

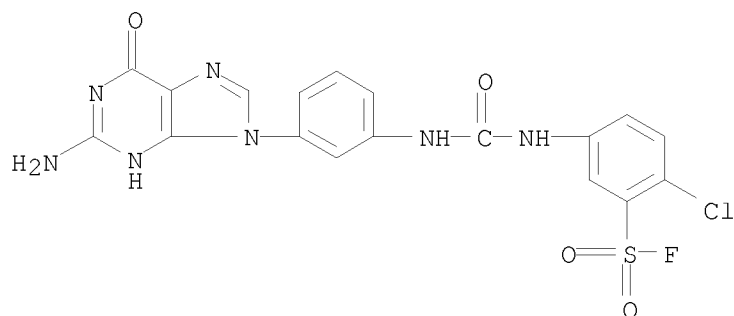


RN 33873-40-4 CAPLUS

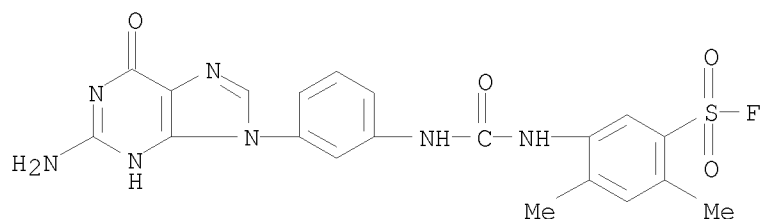
CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methyl- (CA INDEX NAME)



RN 33873-41-5 CAPLUS
 CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



RN 33873-42-6 CAPLUS
 CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2,4-dimethyl- (CA INDEX NAME)



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L4 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:478248 CAPLUS

DOCUMENT NUMBER: 87:78248

ORIGINAL REFERENCE NO.: 87:12365a,12368a

TITLE: Quantitative structure-activity studies. Part III.
 Use of van der Waals volume in structure-activity studies

AUTHOR(S): Moriguchi, Ikuo; Kanada, Yayoi

CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1977), 25(5), 926-35

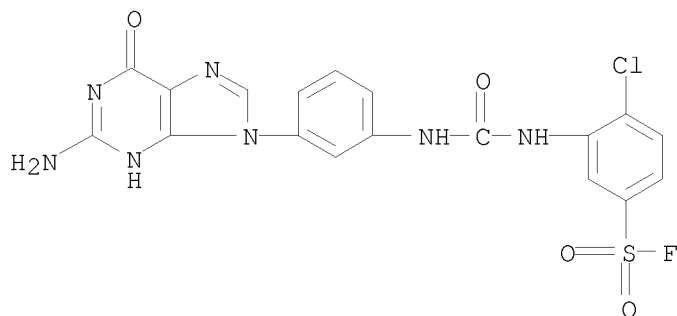
CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

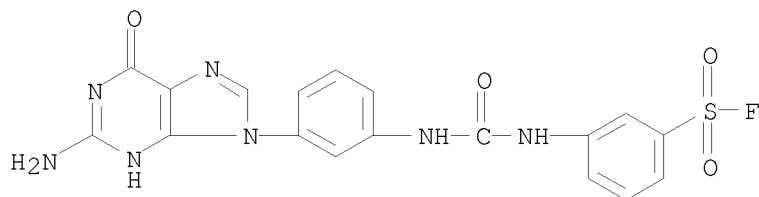
LANGUAGE: English

AB Several structure-activity data, which had been analyzed using molar attraction constant, partition coefficient, connectivity index, and molar refraction as a parameter for drug structure, were reexamd. by the use of van der Waals volume (VW). These data included in vivo antibacterial activity of penicillins, tadpole narcosis with miscellaneous compds., inhibition of neuraminidase by dihydroisoquinolines, fungus toxicity with miscellaneous mols., inhibition of xanthine oxidase by phenylguanines, and tuberculostatic activity of isoniazid derivs. In all cases, very significant correlations were found by regression anal. These findings supported the generality of the use of VW to analyze and predict biol. activity relating to mol. structure.

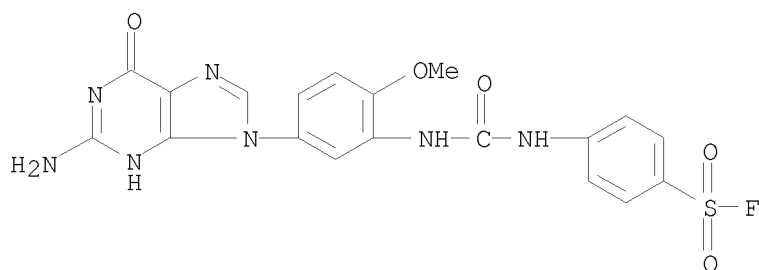
IT 20566-66-9 21318-99-0 21864-31-3
 21864-34-6 21864-35-7 21864-36-8
 21864-38-0 21952-25-0
 RL: BIOL (Biological study)
 (xanthine oxidase inhibition by, van der Waals volume in determination of)
 RN 20566-66-9 CAPLUS
 CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)



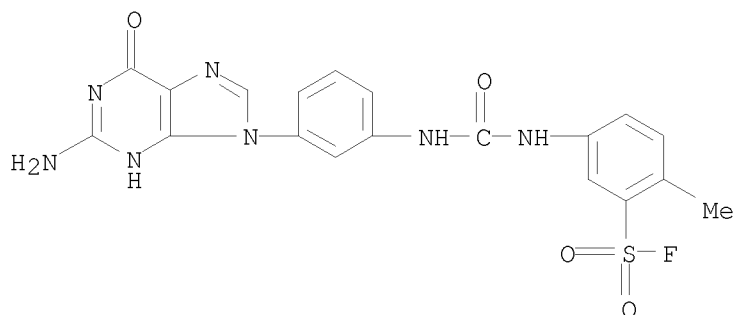
RN 21318-99-0 CAPLUS
 CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



RN 21864-31-3 CAPLUS
 CN Benzenesulfonyl fluoride, 4-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)

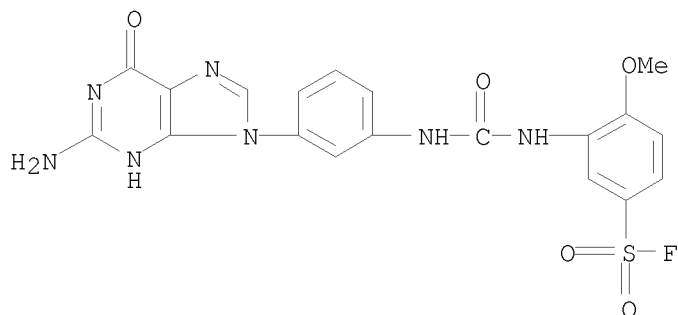


RN 21864-34-6 CAPLUS
 CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)



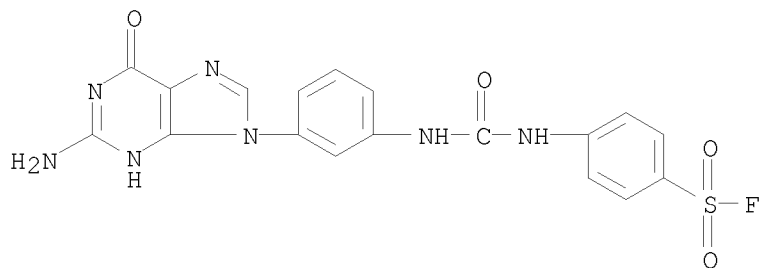
RN 21864-35-7 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)



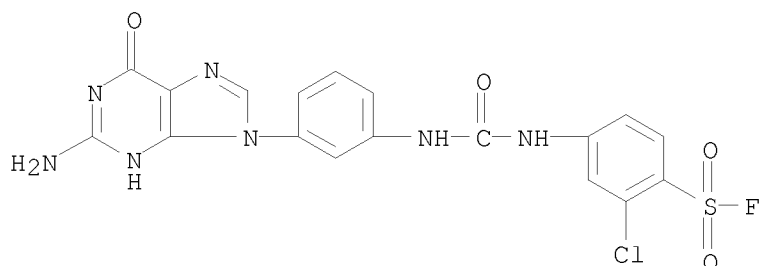
RN 21864-36-8 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)

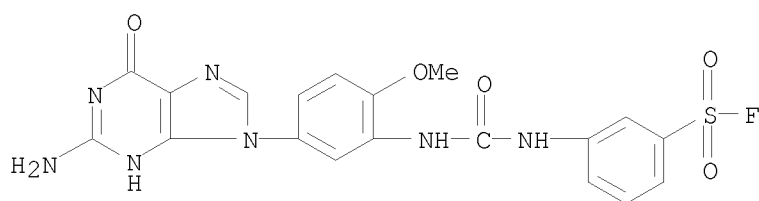


RN 21864-38-0 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



RN 21952-25-0 CAPLUS
 CN Benzenesulfonyl fluoride, 3-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



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L4 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:833039 CAPLUS

DOCUMENT NUMBER: 123:228202

ORIGINAL REFERENCE NO.: 123:40767a, 40770a

TITLE: Pyrazolopyrimidine derivatives as inhibitors of cGMP-specific PDE

INVENTOR(S): Dumaitre, Bernard Andre; Dodic, Nerina

PATENT ASSIGNEE(S): Laboratoires Glaxo SA, Fr.

SOURCE: Eur. Pat. Appl., 34 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

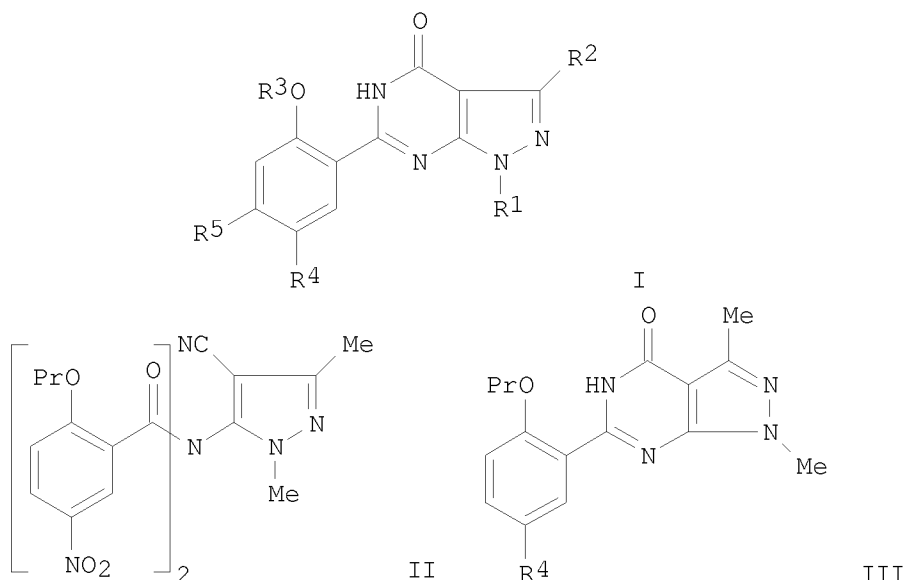
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 636626	A1	19950201	EP 1994-202083	19940718
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07070128	A	19950314	JP 1994-188893	19940719
PRIORITY APPLN. INFO.:			GB 1993-15017	A 19930720
OTHER SOURCE(S):			CASREACT 123:228202; MARPAT 123:228202	

GI



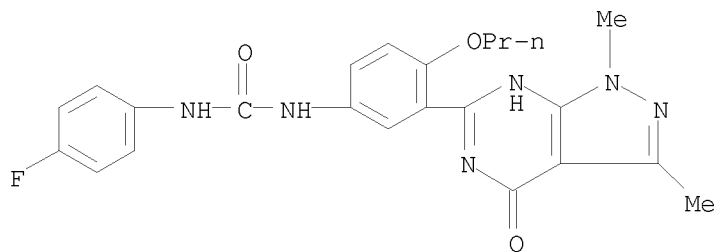
AB Title derivs. I and their salts and solvates are described [in which R1 = arylmethyl or (fluoro)alkyl; R2 = Me; R3 = alkyl; R4 = NO₂, cyano, alkoxy, C(:X)NR₆R₇, NR₈R₉, (CH₂)_mNR₁₀C(:Y)R₁₁, (un)substituted thienyl, thiazolyl, or 1,2,4-triazolyl; or when R1 = arylmethyl or fluoroalkyl then R4 may also = H; R5, R6, R8, R10, R13, R15, R17 = H or alkyl; R7 = H, amino, OH, alkyl, aryl, arylalkyl; R9 = H, alkyl, SO₂R₁₂, CO₂R₁₂, C(:NCN)SR₁₂ or C(:NCN)NR₁₃R₁₄; R11 = (halo)alkyl, aryl, arylalkyl, thienyl, NR₁₅R₁₆, CH₂NR₁₇R₁₈; or R10R₁₁, R10R₁₅ = A(CH₂)_n; R12 = alkyl, aryl, arylalkyl; R14 = H, alkyl, aryl, arylalkyl; or NR₁₃R₁₄, NR₁₅R₁₆, NR₁₇R₁₈ = morpholino, (alkyl)piperazino; R16 = H, alkyl, aryl, arylalkyl, CO₂R₁₂, CH₂CO₂R₁₂; R18 = H, alkyl, aryl, arylalkyl, COR₁₂; A = CH₂, CO; m = 0-1; n = 1-3; X = S, NH, and also O when R7 = amino; Y = O, S; R4 cannot = NO₂ or NH₂ when R1 = alkyl and R5 = H]. The compds. are potent and selective inhibitors of cyclic guanosine 3',5'-monophosphate specific phosphodiesterase (cGMP-specific PDE) and are useful in a variety of therapeutic areas, including the treatment of cardiovascular disorders. For example, cyclocondensation of MeNHNH₂ with Me(EtO)C:C(CN)₂ gave 5-amino-4-cyano-1,3-dimethylpyrazole, which reacted with 2 equiv 2-propoxy-5-nitrobenzoyl chloride to give cyanopyrazole intermediate II. Cyclization of II in a mixture of 30% H₂O₂ and 0.5N NaOH at 90° gave title compound III (R4 = NO₂), which underwent hydrogenation to give III (R4 = NH₂) and then mesylation with MeSO₂Cl to give III (R4 = NHSO₂Me). The latter 2 examples of III had IC₅₀ of 1-10 nM against the title enzyme, vs. 200 nM for the known inhibitor zaprinast.

IT 168464-51-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidine derivs. as inhibitors of cGMP-specific PDE)

RN 168464-51-5 CAPLUS

CN Urea, N-[3-(4,5-dihydro-1,3-dimethyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)-4-propoxyphenyl]-N'-(4-fluorophenyl)- (CA INDEX NAME)



=> d ibib abs hitstr 15

L4 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:175895 CAPLUS

DOCUMENT NUMBER: 124:249654

ORIGINAL REFERENCE NO.: 124:45901a,45904a

TITLE: Synthesis and Cyclic GMP Phosphodiesterase Inhibitory Activity of a Series of 6-Phenylpyrazolo[3,4-d]pyrimidones

AUTHOR(S): Dumaitre, Bernard; Dodic, Nerina

CORPORATE SOURCE: Glaxo Wellcome Centre de Recherches, Les Ulis, 91951, Fr.

SOURCE: Journal of Medicinal Chemistry (1996), 39(8), 1635-44
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of 6-phenylpyrazolo[3,4-d]pyrimidones is described which are specific inhibitors of cGMP specific (type V) phosphodiesterase. Enzymic and cellular activity as well as in vivo oral antihypertensive activity are evaluated. A n-propoxy group at the 2-position of the Ph ring is necessary for activity. A series of products substituted at the 5-position in addition to the 2-n-propoxy was prepared and evaluated. This position can accommodate many unrelated groups. Amino derivs. were very potent but lacked metabolic stability. Substitution by carbon-linked small heterocycles provided both high levels of activity and stability. Cellular activity very often correlated with in vivo activity. Among the compds., 1,3-dimethyl-6-(2-propoxy-5-methanesulfonamidophenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one and 1-ethyl-3-methyl-6-(2-propoxy-5-(4-methylthiazol-2-yl)phenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one displayed outstanding in vivo activities at 5 mg/kg/os and good metabolic stabilities.

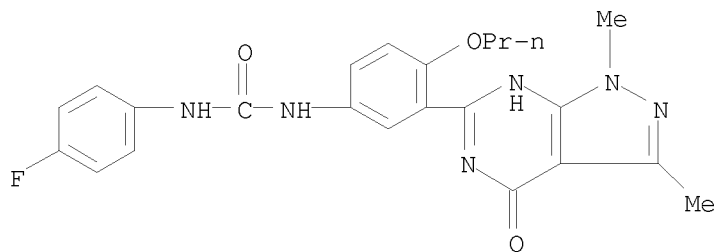
IT 168464-51-5P

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(synthesis and cyclic GMP phosphodiesterase inhibitory activity of phenylpyrazolopyrimidones)

RN 168464-51-5 CAPLUS

CN Urea, N-[3-(4,5-dihydro-1,3-dimethyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)-4-propoxyphenyl]-N'-(4-fluorophenyl)- (CA INDEX NAME)



=> d ibib abs hitstr 14

L4 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:208278 CAPLUS

DOCUMENT NUMBER: 134:252353

TITLE: Preparation of pyrazolopyrimidines as protein kinase inhibitors

INVENTOR(S): Hirst, Gavin C.; Calderwood, David; Wishart, Neil; Rafferty, Paul; Ritter, Kurt; Arnold, Lee D.; Friedman, Michael M.

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 527 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

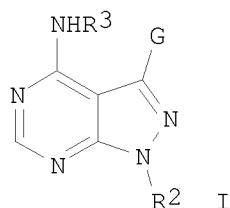
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

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AU 2000074950	A	20010417	AU 2000-74950	20000915
AU 780052	B2	20050224		
EP 1212327	A2	20020612	EP 2000-963554	20000915
EP 1212327	B1	20030820		
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BR 2000014073	A	20020716	BR 2000-14073	20000915
JP 2003509428	T	20030311	JP 2001-523406	20000915
AT 247657	T	20030915	AT 2000-963554	20000915
PT 1212327	T	20040130	PT 2000-963554	20000915
ES 2207552	T3	20040601	ES 2000-963554	20000915
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TW 230709	B	20050411	TW 2000-89119064	20000916
IN 2002MN00310	A	20080815	IN 2002-MN310	20020313
ZA 2002002123	A	20030617	ZA 2002-2123	20020314
MX 2002PA02898	A	20031014	MX 2002-PA2898	20020314

NO 2002001328	A	20020521	NO 2002-1328	20020318
BG 106586	A	20030131	BG 2002-106586	20020405
HK 1050355	A1	20041015	HK 2002-108955	20021210
PRIORITY APPLN. INFO.:			US 1999-154620P	P 19990917
			WO 2000-US25468	W 20000915

OTHER SOURCE(S): MARPAT 134:252353
GI

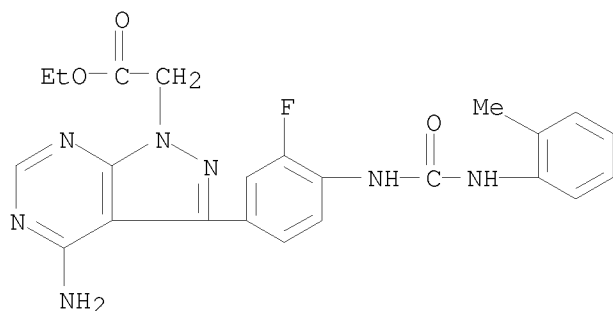


AB The title compds. [I; G = substituted Ph; R2 = BE; B = (un)substituted cycloalkyl, azacycloalkyl, etc.; E = (un)substituted azacycloalkyl, azacycloalkylcarbonyl, etc.; R3 = H, OH, alkyl, alkoxy] which inhibit one or more protein kinase (such as FGFR, PDGFR, KDR, Tie-2, Lck, Fyn, Blk, Lyn, Src, and cdc2) activity, were prepared and formulated. E.g., a multi-step synthesis of I [G = 4-phenoxyphenyl; R2 = 1-benzyl-4-piperidinyl; R3 = H] was described. Biol. data for compds. I were given.

IT 330790-95-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrazolopyrimidines as protein kinase inhibitors)

RN 330790-95-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-acetic acid, 4-amino-3-[3-fluoro-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)



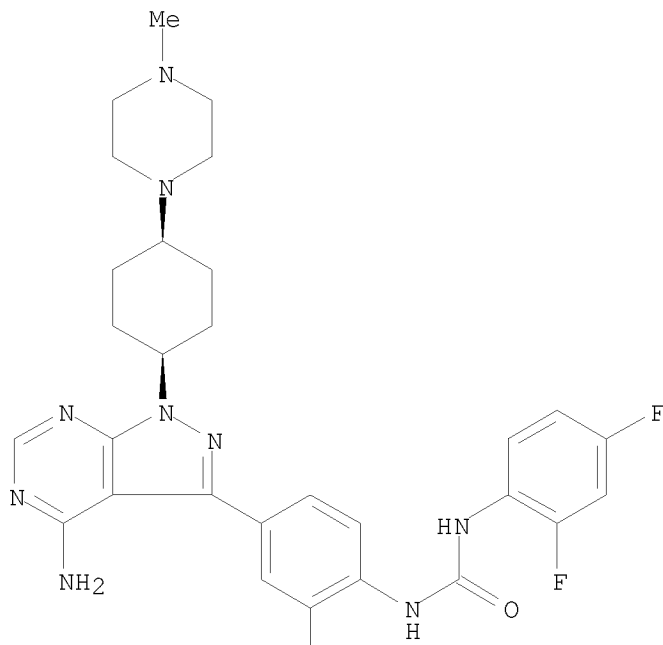
IT 330788-46-0P 330788-48-2P 330788-50-6P
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330791-01-0P 330791-02-1P 330791-06-5P
330791-07-6P 330791-74-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidines as protein kinase inhibitors)

RN 330788-46-0 CAPLUS

CN Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(2,4-difluorophenyl)-
(CA INDEX NAME)

Relative stereochemistry.

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RN 330788-48-2 CAPLUS

CN Urea, N-[4-[4-amino-1-[trans-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methoxyphenyl)-, acetate (1:1) (CA INDEX NAME)

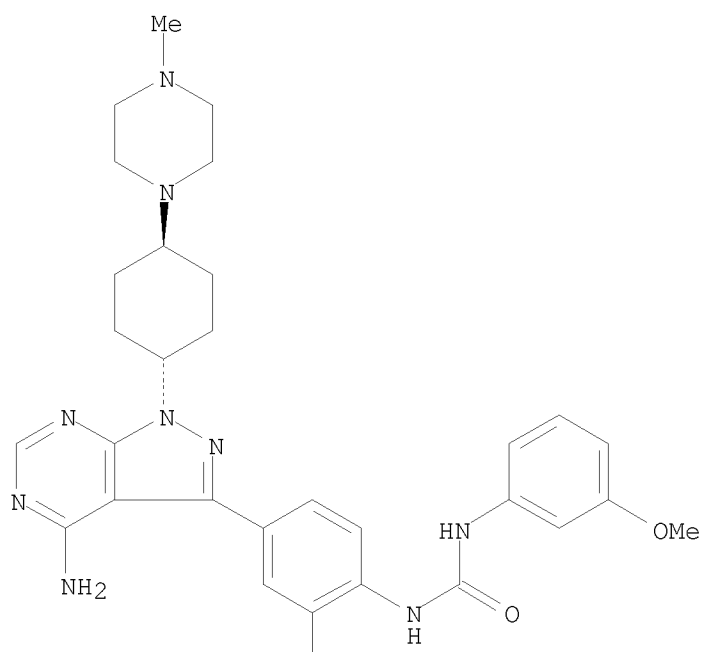
CM 1

CRN 330788-47-1

CMF C30 H36 F N9 O2

Relative stereochemistry.

PAGE 1-A

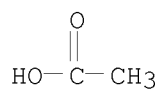


PAGE 2-A



CM 2

CRN 64-19-7
CMF C2 H4 O2



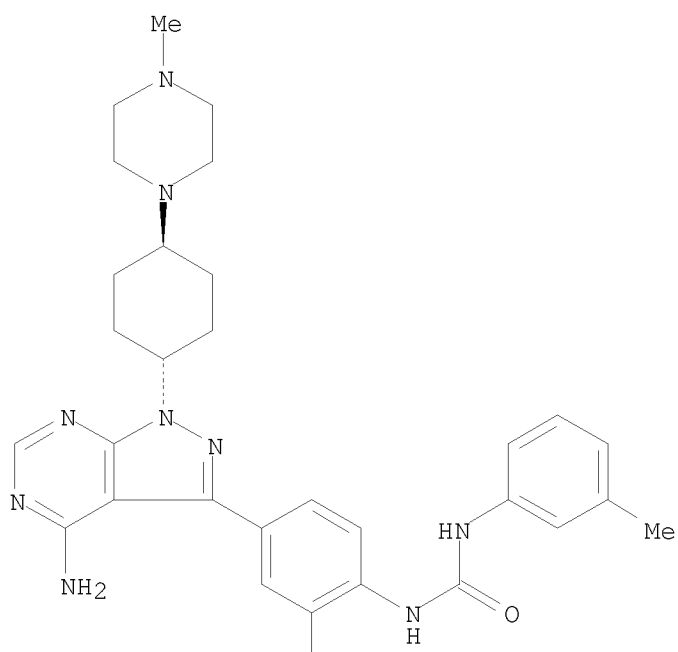
RN 330788-50-6 CAPLUS
CN Urea, N-[4-[4-amino-1-[trans-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

CRN 330788-49-3
CMF C30 H36 F N9 O

Relative stereochemistry.

PAGE 1-A

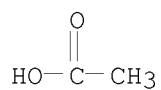


PAGE 2-A



CM 2

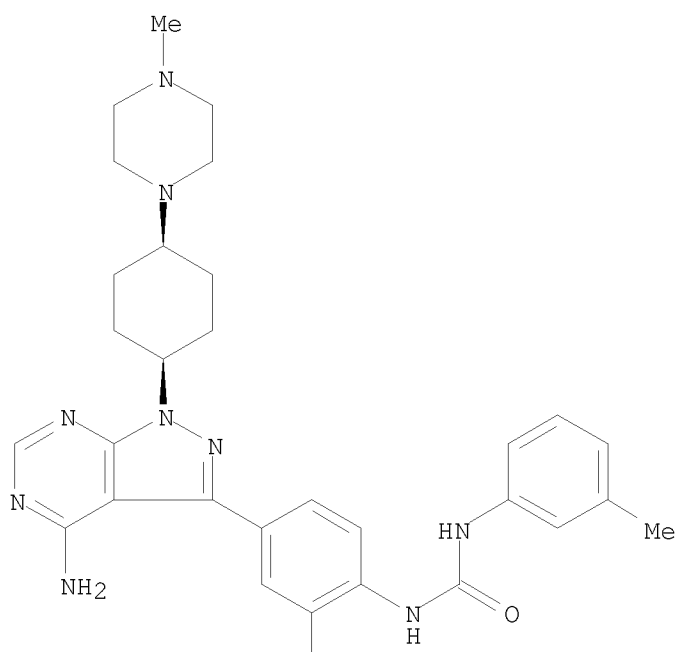
CRN 64-19-7
CMF C2 H4 O2



RN 330788-51-7 CAPLUS
CN Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



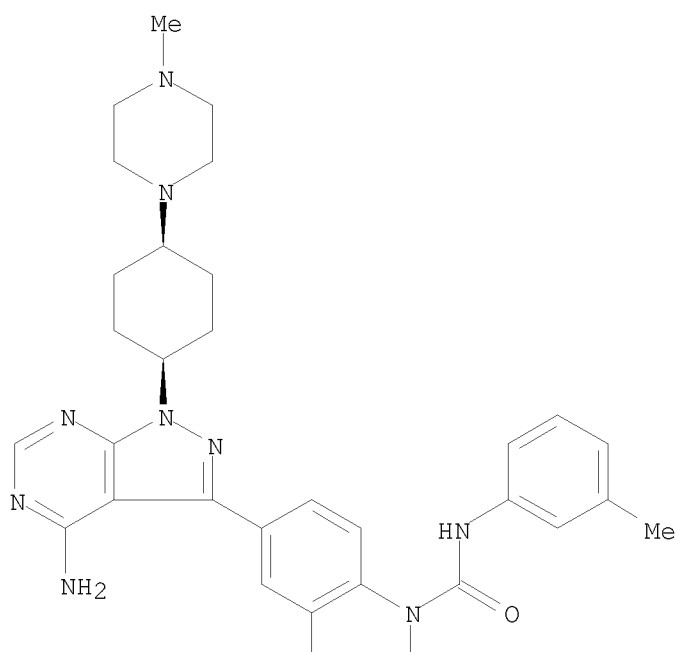
PAGE 2-A

F

RN 330788-52-8 CAPLUS
CN Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N-ethyl-N'-(3-methylphenyl)-
(CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



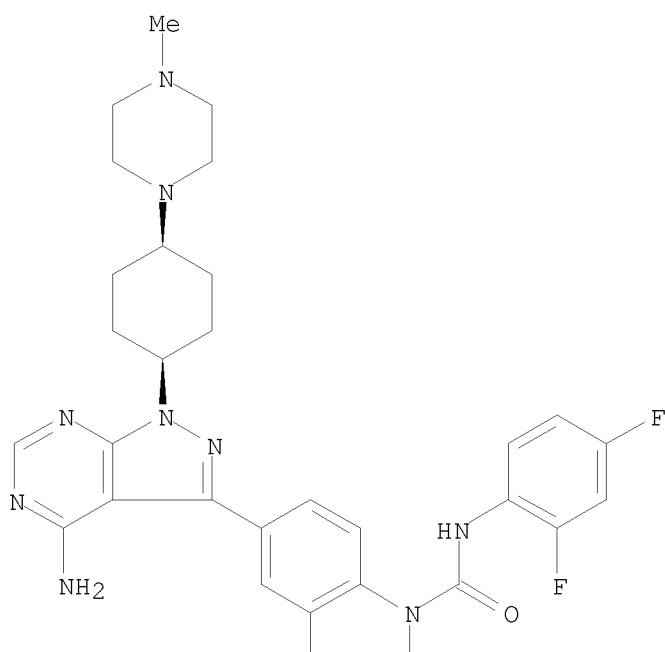
PAGE 2-A



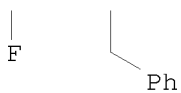
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CN Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(2,4-difluorophenyl)-N-(phenylmethyl)- (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

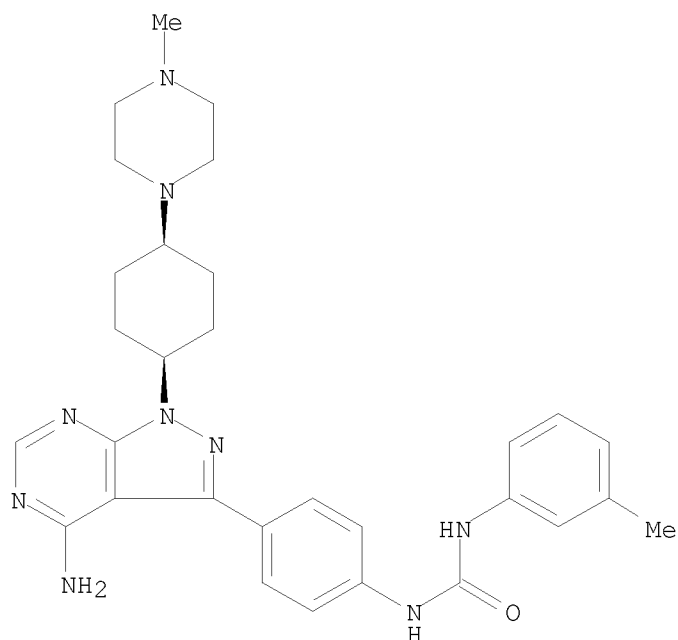


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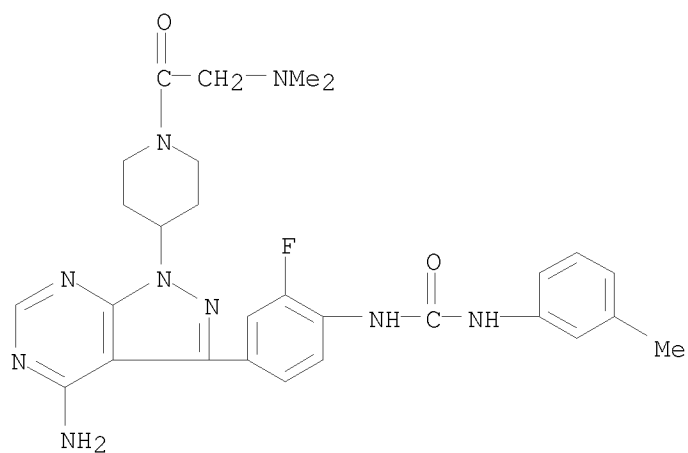


RN 330788-54-0 CAPLUS
CN Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)

Relative stereochemistry.



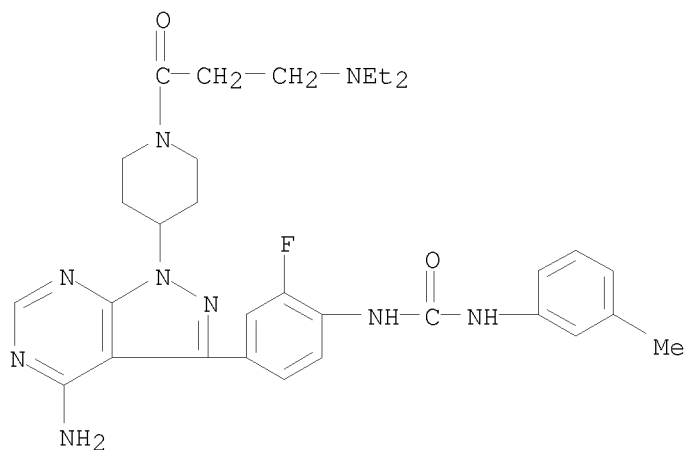
RN 330788-55-1 CAPLUS
 CN Urea, N-[4-[4-amino-1-[1-[2-(dimethylamino)acetyl]-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



RN 330788-57-3 CAPLUS
 CN Urea, N-[4-[4-amino-1-[1-[3-(diethylamino)-1-oxopropyl]-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, acetate (1:1) (CA INDEX NAME)

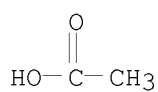
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CRN 330788-56-2
 CMF C31 H38 F N9 O2

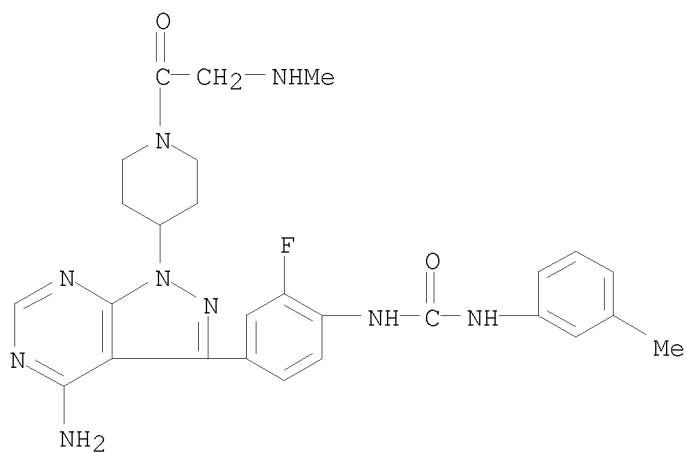


CM 2

CRN 64-19-7
CMF C2 H4 O2



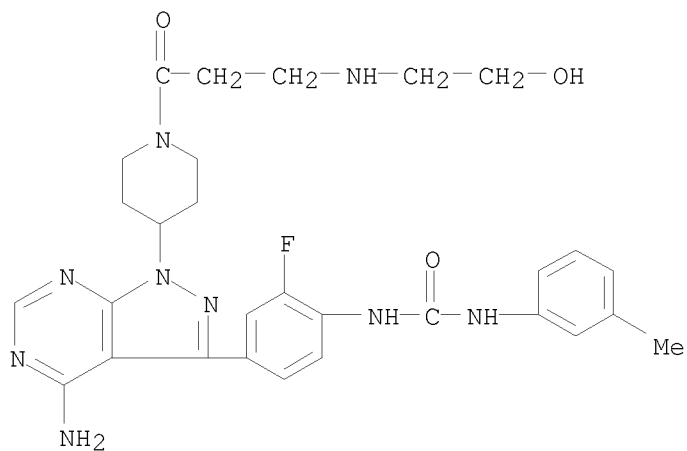
RN 330788-58-4 CAPLUS
CN Urea, N-[4-[4-amino-1-[1-[2-(methylamino)acetyl]-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



RN 330788-60-8 CAPLUS
CN Urea, N-[4-[4-amino-1-[1-[3-[(2-hydroxyethyl)amino]-1-oxopropyl]-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, acetate (1:1) (CA INDEX NAME)

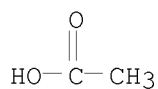
CM 1

CRN 330788-59-5
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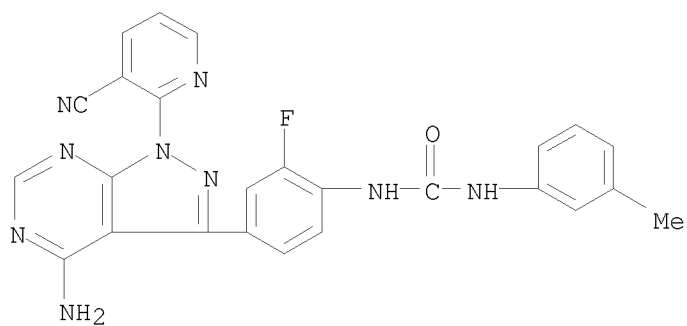


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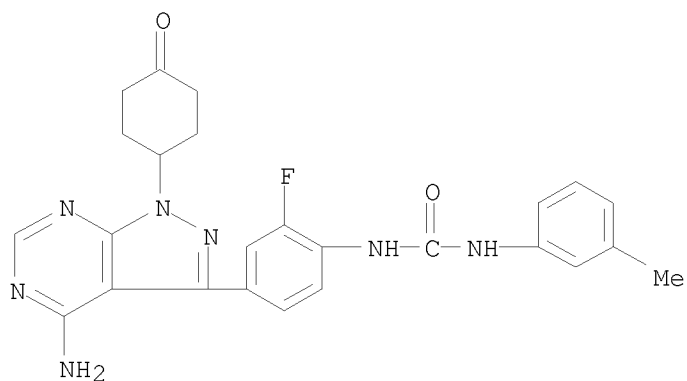
CRN 64-19-7
CMF C2 H4 O2



RN 330788-70-0 CAPLUS
CN Urea, N-[4-[4-amino-1-(3-cyano-2-pyridinyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)

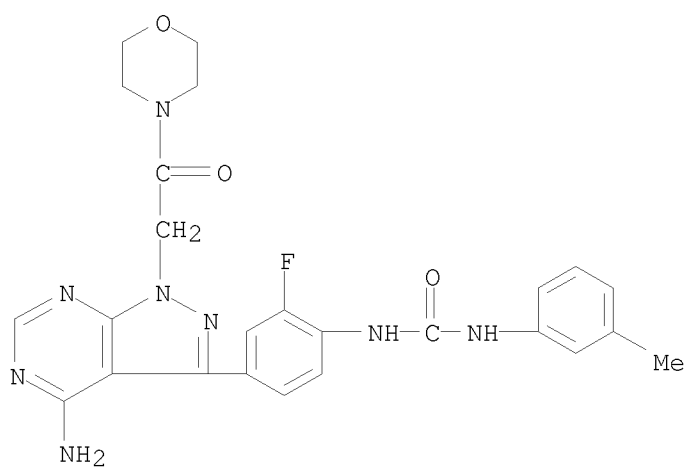


RN 330788-91-5 CAPLUS
CN Urea, N-[4-[4-amino-1-(4-oxocyclohexyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



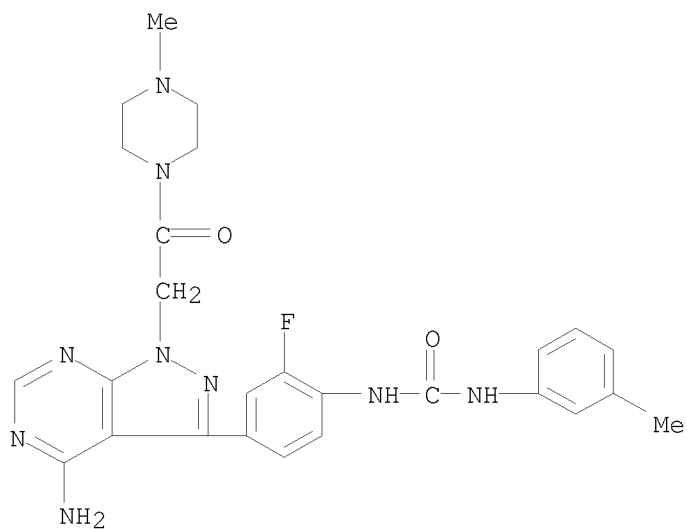
RN 330790-96-0 CAPLUS

CN Urea, N-[4-[4-amino-1-[2-(4-morpholinyl)-2-oxoethyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



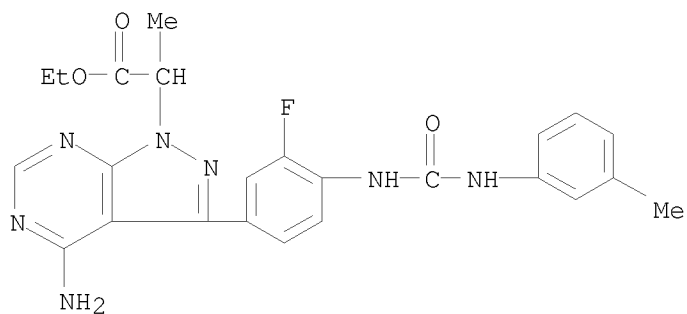
RN 330790-97-1 CAPLUS

CN Urea, N-[4-[4-amino-1-[2-(4-methyl-1-piperazinyl)-2-oxoethyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



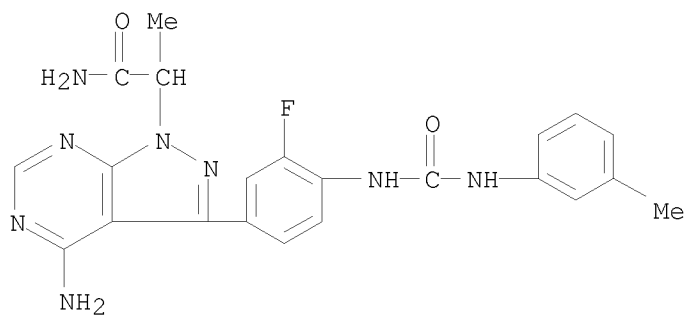
RN 330791-01-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-acetic acid, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-α-methyl-, ethyl ester
(CA INDEX NAME)



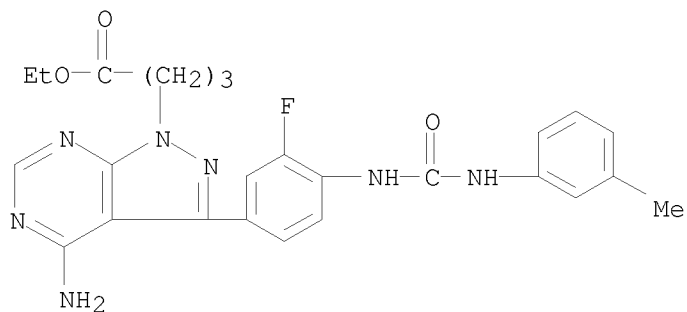
RN 330791-02-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-acetamide, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-α-methyl- (CA INDEX NAME)



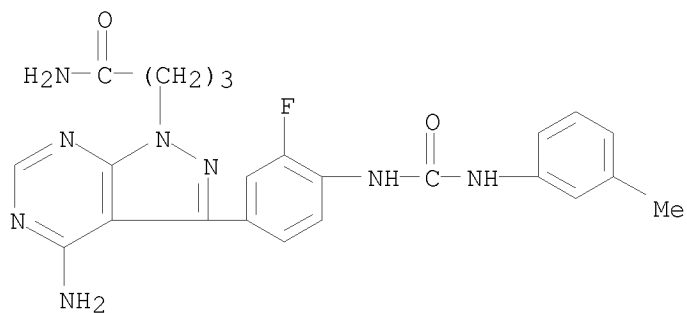
RN 330791-06-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-butanoic acid, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)



RN 330791-07-6 CAPLUS

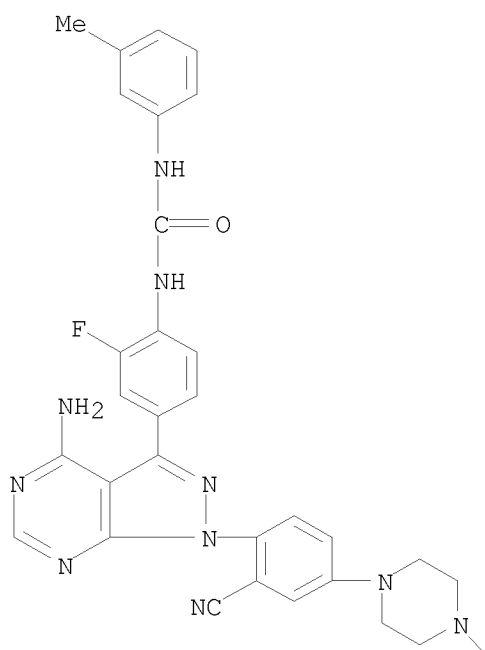
CN 1H-Pyrazolo[3,4-d]pyrimidine-1-butanamide, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]- (CA INDEX NAME)



RN 330791-74-7 CAPLUS

CN Urea, N-[4-[4-amino-1-[2-cyano-4-(4-methyl-1-piperazinyl)phenyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)

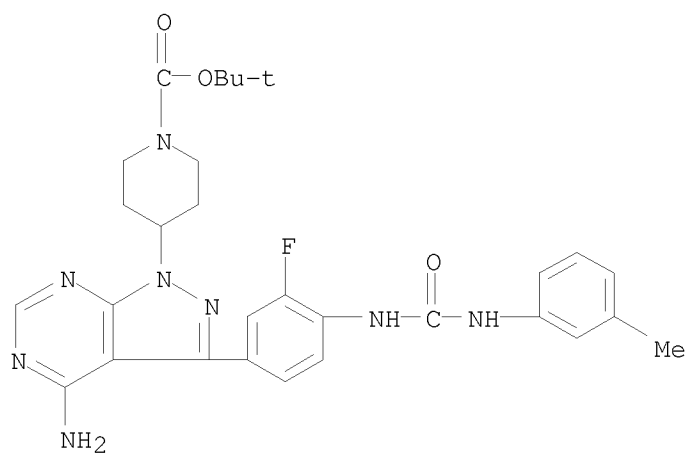
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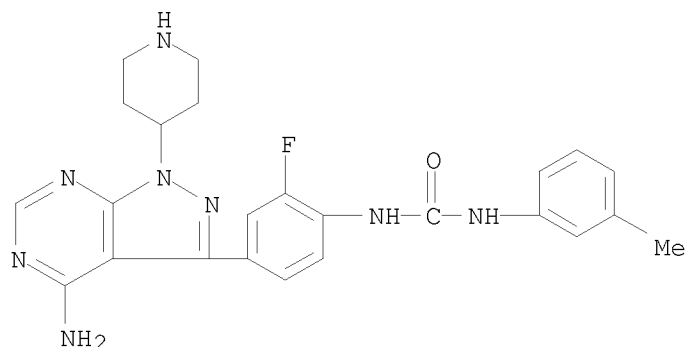
PAGE 2-A



IT 330793-24-3P 330793-25-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of pyrazolopyrimidines as protein kinase inhibitors)
 RN 330793-24-3 CAPLUS
 CN 1-Piperidinecarboxylic acid, 4-[4-amino-3-[3-fluoro-4-[[[(3-
 methylphenyl)amino]carbonyl]amino]phenyl]-1H-pyrazolo[3,4-d]pyrimidin-1-
 yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 330793-25-4 CAPLUS
 CN Urea, N-[4-[4-amino-1-(4-piperidiny1)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, hydrochloride (1:2) (CA INDEX NAME)



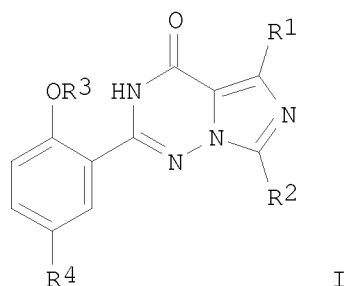
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=> d ibib abs hitstr 13

L4 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:657494 CAPLUS
 DOCUMENT NUMBER: 135:211060
 TITLE: Preparation of 2-phenylimidazotriazinones as
 cGMP-metabolizing phosphodiesterase inhibitors
 INVENTOR(S): Niewoehner, Ulrich; Es-Sayed, Mazen; Lampe, Thomas;
 Haning, Helmut; Schmidt, Gunther; Schlemmer,
 Karl-Heinz; Bischoff, Erwin; Dembowsky, Klaus;
 Perzborn, Elisabeth
 PATENT ASSIGNEE(S): Bayer A.-G., Germany
 SOURCE: Ger. Offen., 154 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10010067	A1	20010906	DE 2000-10010067	20000302
CA 2401834	A1	20010907	CA 2001-2401834	20010220
WO 2001064677	A1	20010907	WO 2001-EP1871	20010220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1280805	A1	20030205	EP 2001-911663	20010220
EP 1280805	B1	20050209		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR						
BR	2001008853	A	20030429	BR	2001-8853	20010220
JP	2003525293	T	20030826	JP	2001-564174	20010220
AT	288916	T	20050215	AT	2001-911663	20010220
PT	1280805	T	20050630	PT	2001-911663	20010220
ES	2236190	T3	20050716	ES	2001-911663	20010220
AU	2001240637	B2	20060309	AU	2001-240637	20010220
ZA	2002006217	A	20030805	ZA	2002-6217	20020805
IN	2002MN01095	A	20040529	IN	2002-MN1095	20020813
MX	2002PA08505	A	20030128	MX	2002-PA8505	20020830
US	20040097498	A1	20040520	US	2003-220560	20030206
US	6878708	B2	20050412			
HK	1055423	A1	20060825	HK	2003-106960	20030926
US	20050267112	A1	20051201	US	2005-30605	20050105
US	7098207	B2	20060829			
PRIORITY APPLN. INFO.:				DE	2000-10010067	A 20000302
				WO	2001-EP1871	W 20010220
				US	2003-220560	A1 20030206
OTHER SOURCE(S):				MARPAT 135:211060		
GI						



AB Title compds. [I; R1 = alkyl; R2 = cycloalkyl, alkyl; R3 = alkyl; R4 = NHSO2R5, N(SO2R6)SO2R7, etc.; R5, R6, R7 = (substituted) vinyl, alkyl, aryl; or R5 = quinolyl, (substituted) heteroaryl, etc.], were prepared as phosphodiesterase I and phosphodiesterase V inhibitors (no data). Thus, 2-(5-amino-2-ethoxyphenyl)-5-methyl-7-cyclopentyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one (preparation given) in THF was treated at 5° with 4-morpholinocarbonyl chloride in THF followed by stirring overnight at room temperature to give 98%

2-[2-ethoxy-5-(4-morpholinocarbonylamino)phenyl]-5-methyl-7-cyclopentyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one.

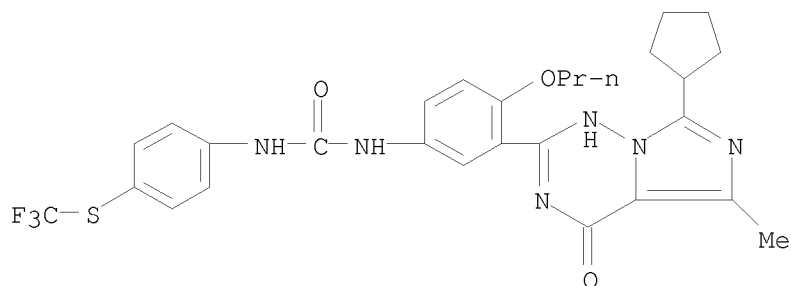
IT 358389-16-9P 358389-17-0P 358389-31-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phenylimidazotriazinones as cGMP-metabolizing phosphodiesterase inhibitors)

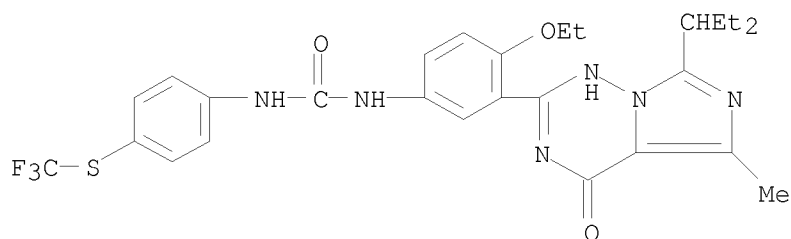
RN 358389-16-9 CAPLUS

CN Urea, N-[3-(7-cyclopentyl-1,4-dihydro-5-methyl-4-oxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-propoxyphenyl]-N'-[4-[(trifluoromethyl)thio]phenyl]- (CA INDEX NAME)



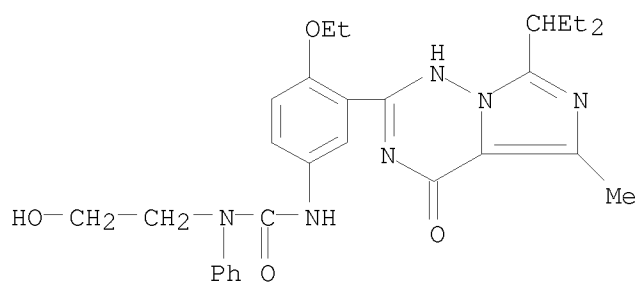
RN 358389-17-0 CAPLUS

CN Urea, N-[4-ethoxy-3-[7-(1-ethylpropyl)-1,4-dihydro-5-methyl-4-oxoimidazo[5,1-f][1,2,4]triazin-2-yl]phenyl]-N'-[4-[(trifluoromethyl)thio]phenyl]- (CA INDEX NAME)



RN 358389-31-8 CAPLUS

CN Urea, N'-[4-ethoxy-3-[7-(1-ethylpropyl)-1,4-dihydro-5-methyl-4-oxoimidazo[5,1-f][1,2,4]triazin-2-yl]phenyl]-N-(2-hydroxyethyl)-N-phenyl- (CA INDEX NAME)



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L4 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:407945 CAPLUS

DOCUMENT NUMBER: 138:49367

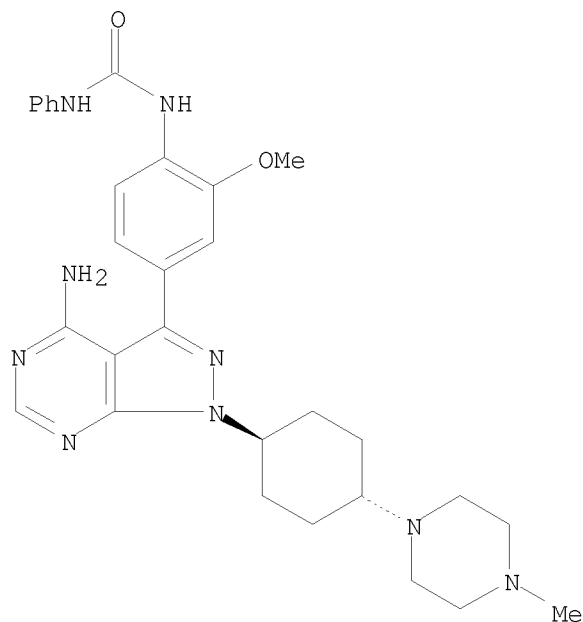
TITLE: Pyrazolo[3,4-d]pyrimidines containing an extended 3-substituent as potent inhibitors of Lck - a selectivity insight

AUTHOR(S): Burchat, Andrew F.; Calderwood, David J.; Friedman, Michael M.; Hirst, Gavin C.; Li, Biqin; Rafferty, Paul; Ritter, Kurt; Skinner, Barbara S.

CORPORATE SOURCE: Abbott Bioresearch Center, Worcester, MA, 01605-5314, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002),
12(12), 1687-1690
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:49367
AB A series of para-substituted 3-Ph pyrazolopyrimidines was synthesized and evaluated as inhibitors of lck. The nature of the substitution affected enzyme selectivity and potency for lck, src, kdr, and tie-2. One of the para-phenoxyphenyl pyrazolopyrimidine analog is an orally active lck inhibitor with a bioavailability of 69% and exhibits an extended duration of action in animal models of T cell inhibition.
IT 479546-21-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(structure-activity relationship of substituted pyrazolopyrimidines as potent inhibitors of Lck)
RN 479546-21-9 CAPLUS
CN Urea, N-[4-[4-amino-1-[trans-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-methoxyphenyl]-N'-phenyl- (CA INDEX NAME)

Relative stereochemistry.



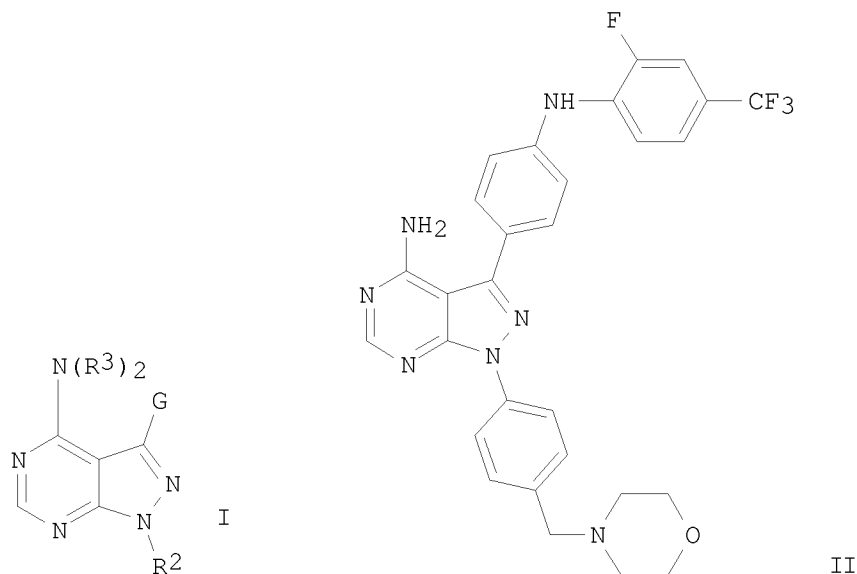
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 11

L4 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:793426 CAPLUS
DOCUMENT NUMBER: 137:310925
TITLE: Preparation of 3-(azahetero)aryl-1H-pyrazolo[3,4-d]pyrimidin-3-amines as protein kinase inhibitors with antiangiogenic properties
INVENTOR(S): Hirst, Gavin C.; Rafferty, Paul; Ritter, Kurt;

Calderwood, David; Wishart, Neil; Arnold, Lee D.;
 Friedman, Michael M.
 PATENT ASSIGNEE(S): Abbott G.m.b.H. & Co. K.-G., Germany
 SOURCE: PCT Int. Appl., 867 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002080926	A1	20021017	WO 2002-US9104	20020322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20020156081	A1	20021024	US 2001-815310	20010322
US 6921763	B2	20050726		
CA 2440724	A1	20021017	CA 2002-2440724	20020322
AU 2002316030	A1	20021021	AU 2002-316030	20020322
EP 1385524	A1	20040204	EP 2002-746301	20020322
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004531513	T	20041014	JP 2002-578965	20020322
BR 2002005889	A	20041109	BR 2002-5889	20020322
NO 2003004176	A	20031121	NO 2003-4176	20030919
MX 2003PA08561	A	20040630	MX 2003-PA8561	20030922
IN 2003MN00935	A	20050429	IN 2003-MN935	20031003
PRIORITY APPLN. INFO.:			US 2001-815310	A 20010322
			US 1999-154620P	P 19990917
			US 2000-663780	A2 20000915
			WO 2002-US9104	W 20020322
OTHER SOURCE(S):			MARPAT 137:310925	
GI				

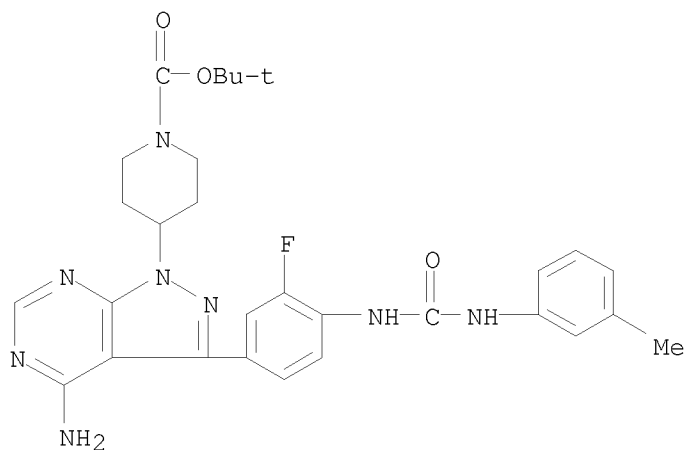


AB Title compds. I [wherein G = (un)substituted 5-6 membered (azahetero)aryl; R2 = H or (un)substituted trityl, cycloalkenyl, azaheteroaryl, or C6H4-4-CH2E; E = (un)substituted alkyl-OR, alkyl-CO2R, alkylheteroaryl, alkylheterocycloalkyl, or alkyl-NR2; R = independently H or (un)substituted (cyclo)alkyl, or aryl(alkyl); R3 = independently H, OH, or (un)substituted alkyl, alkyl-CO, (hetero)aryl-CO, or alkoxy; or racemic diastereomeric mixts., optical isomers, pharmaceutically acceptable salts, prodrugs, and/or biol. active metabolites thereof] were prepared For example, 3-iodo-1H-pyrazolo[3,4-d]pyrimidin-4-amine was coupled with 4-fluorobenzaldehyde in the presence of NaH in DMF to give 4-(4-amino-3-iodo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)benzaldehyde. Treatment of the 3-iodopyrazolopyrimidine with N-[2-methoxy-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-2-fluoro-4-(trifluoromethyl)benzamide, Pd(PPh3)4, and Na2CO3 in H2O afforded the N-[4-(pyrazolopyrimidin-3-yl)phenyl]benzamide. Addition of morpholine to the benzaldehyde in the presence of Na(AcO)3BH in dichloroethane produced II. All exemplified compds. significantly inhibited either FGFR, PDGFR, KDR, Tie-2, Lck, Fyn, Blk, Lyn, or Src at concentration of $\leq 50 \mu\text{M}$. Certain compds. of the invention also significantly inhibited cdc2 or cellular VEGF-induced KDR tyrosine kinase phosphorylation at concns. of $\leq 50 \mu\text{M}$. Thus, I are useful for the treatment of a wide variety of disease states ameliorated by the inhibition of protein tyrosine kinase activity essential for angiogenic processes (no data).

IT 330793-24-3P 330793-25-4P, N-[4-[4-Amino-1-(4-piperidyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea dihydrochloride 471925-82-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of [(hetero)aryl]pyrazolo[3,4-d]pyrimidinamines as protein kinase inhibitors with antiangiogenic properties)

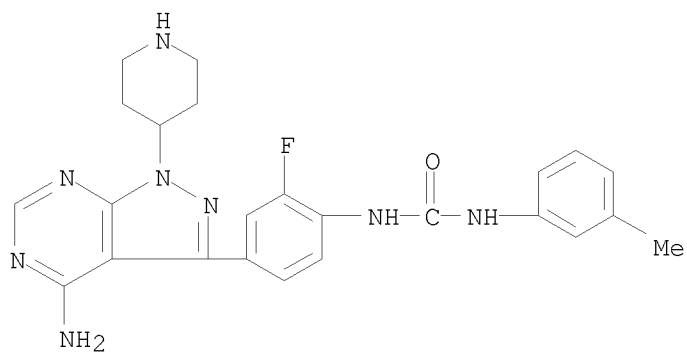
RN 330793-24-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 330793-25-4 CAPLUS

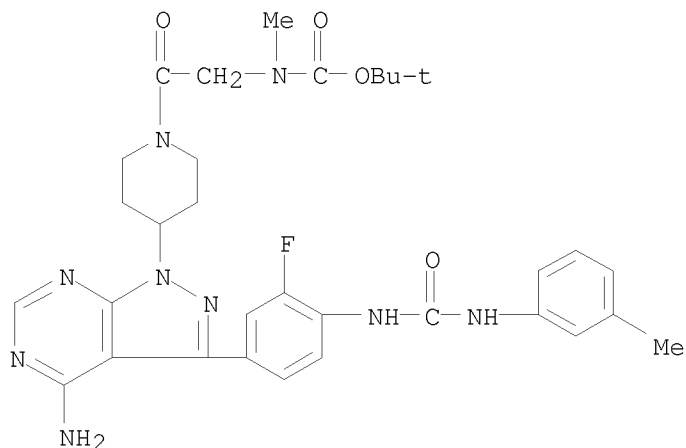
CN Urea, N-[4-[4-amino-1-(4-piperidinyloxy)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

RN 471925-82-3 CAPLUS

CN Carbamic acid, [2-[4-[4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-1-piperidinyloxy]-2-oxoethyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

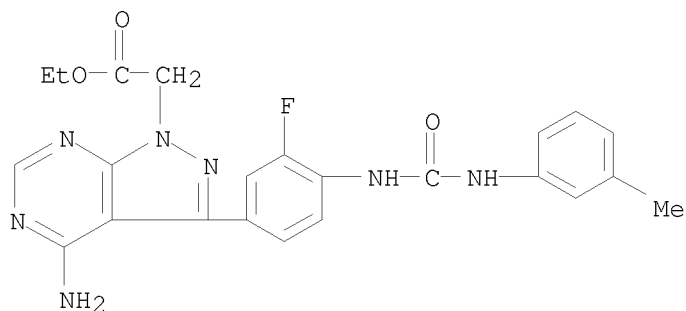


IT 471926-42-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(protein kinase inhibitor; preparation of [(hetero)aryl]pyrazolo[3,4-d]pyrimidinamines as protein kinase inhibitors with antiangiogenic properties)

RN 471926-42-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-acetic acid, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)



IT 330788-46-0P, cis-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(2,4-difluorophenyl)urea 330788-47-1P, trans-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methoxyphenyl)urea 330788-48-2P, trans-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methoxyphenyl)urea monoacetate 330788-50-6P, trans-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea monoacetate 330788-51-7P, cis-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea 330788-52-8P, cis-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N-ethyl-N'-(3-methylphenyl)urea 330788-53-9P, cis-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N-benzyl-N'-(2,4-difluorophenyl)urea 330788-54-0P,

cis-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-(3-methylphenyl)urea 330788-55-1P,
 N-[4-[4-Amino-1-[1-[2-(dimethylamino)acetyl]-4-piperidyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea
 330788-57-3P, N-[4-[4-Amino-1-[1-[3-(diethylamino)propanoyl]-4-piperidyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea monoacetate 330788-58-4P, N-[4-[4-Amino-1-[1-[2-(methylamino)acetyl]-4-piperidyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea 330788-60-8P,
 N-[4-[4-Amino-1-[1-[3-[(2-hydroxyethyl)amino]propanoyl]-4-piperidyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea monoacetate 330788-70-0P 330788-91-5P,
 N-[4-[4-Amino-1-(4-oxocyclohexyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea 330790-96-0P,
 N-[4-[4-Amino-1-(2-morpholino-2-oxoethyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea 330790-97-1P,
 N-[4-[4-Amino-1-[2-(4-methylpiperazino)-2-oxoethyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea
 330791-01-0P 330791-02-1P 330791-06-5P
 330791-07-6P 330791-74-7P, N-[4-[4-Amino-1-[2-cyano-4-(4-methylpiperazino)phenyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

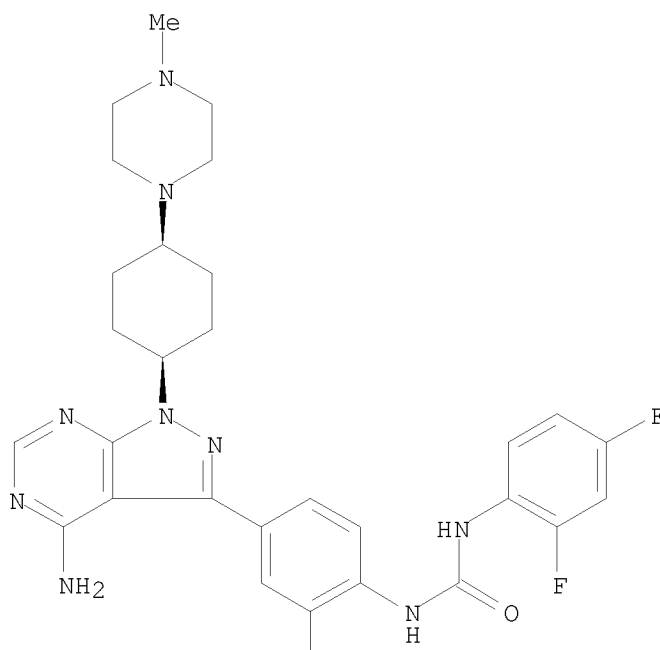
(protein kinase inhibitor; preparation of [(hetero)aryl]pyrazolo[3,4-d]pyrimidinamines as protein kinase inhibitors with antiangiogenic properties)

RN 330788-46-0 CAPLUS

CN Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(2,4-difluorophenyl)-(CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



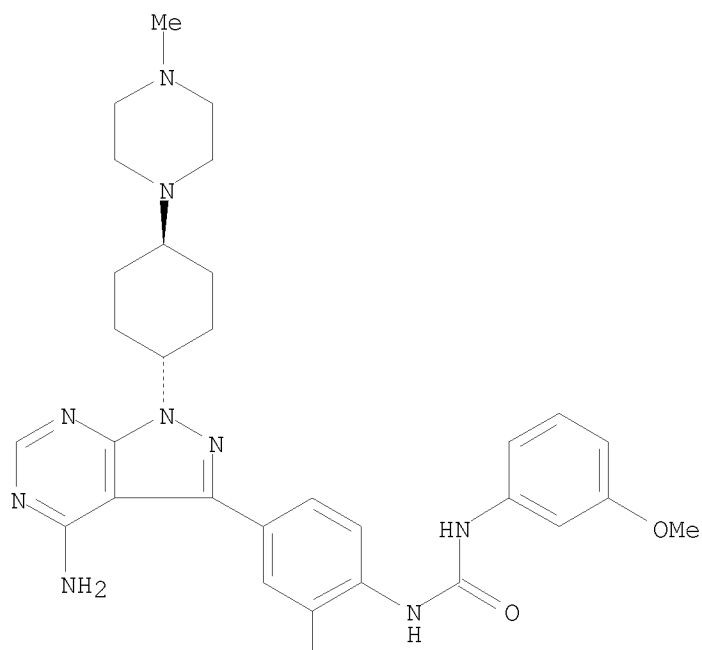
PAGE 2-A

|
F

RN 330788-47-1 CAPLUS
CN Urea, N-[4-[4-amino-1-[trans-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methoxyphenyl)- (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

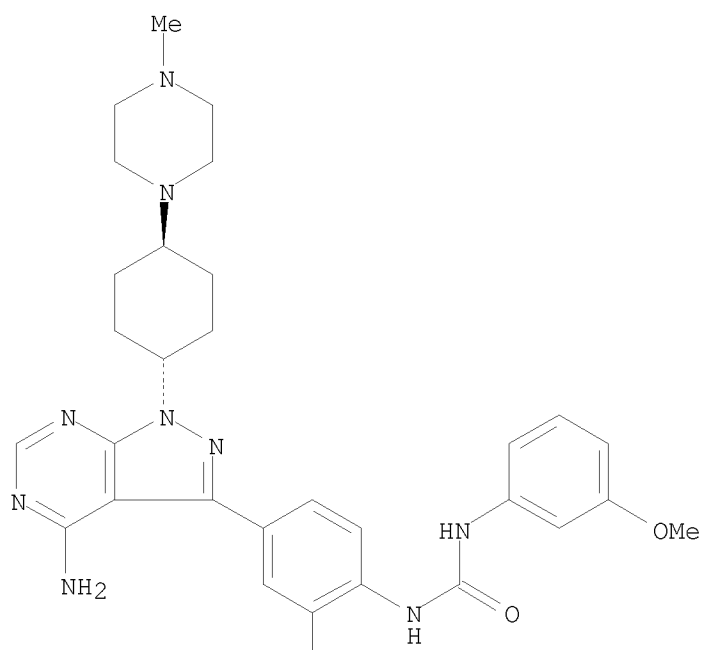
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RN 330788-48-2 CAPLUS
CN Urea, N-[4-[4-amino-1-[trans-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methoxyphenyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

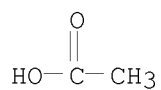
CRN 330788-47-1
CMF C30 H36 F N9 O2

Relative stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2



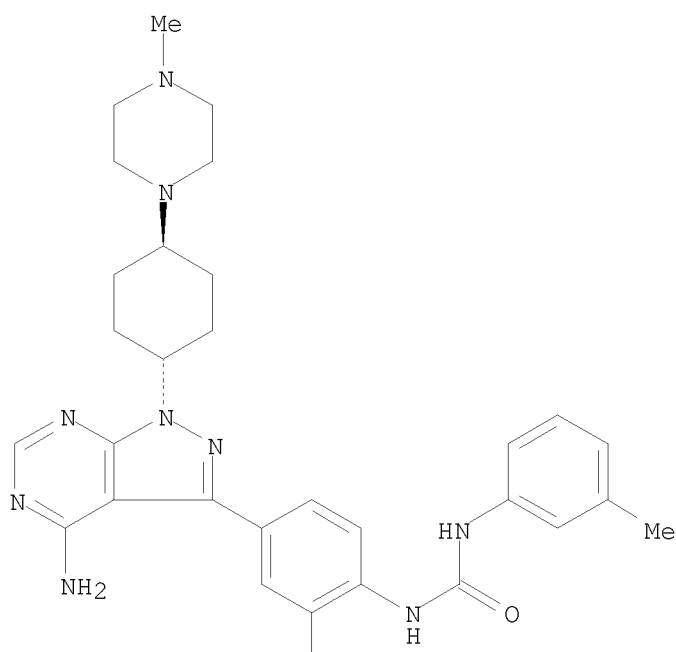
RN 330788-50-6 CAPLUS
CN Urea, N-[4-[4-amino-1-[trans-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

CRN 330788-49-3
CMF C30 H36 F N9 O

Relative stereochemistry.

PAGE 1-A

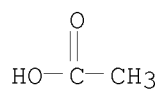


PAGE 2-A



CM 2

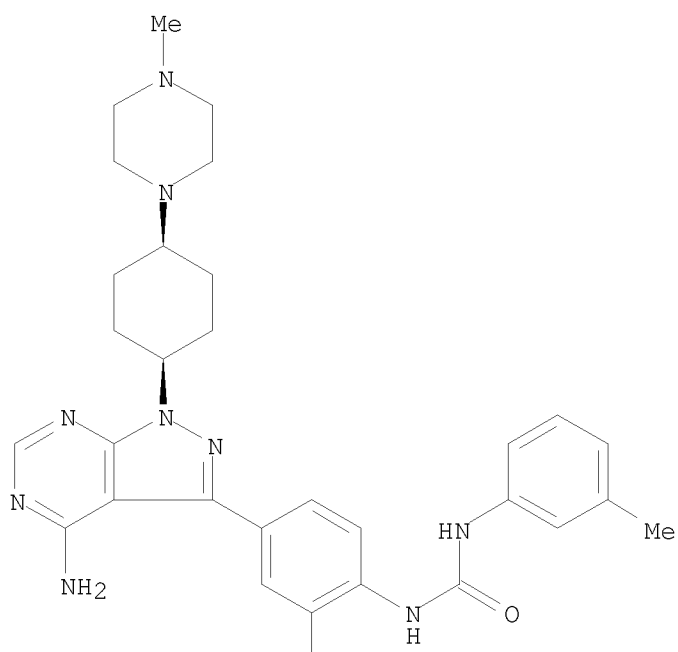
CRN 64-19-7
CMF C2 H4 O2



RN 330788-51-7 CAPLUS
CN Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



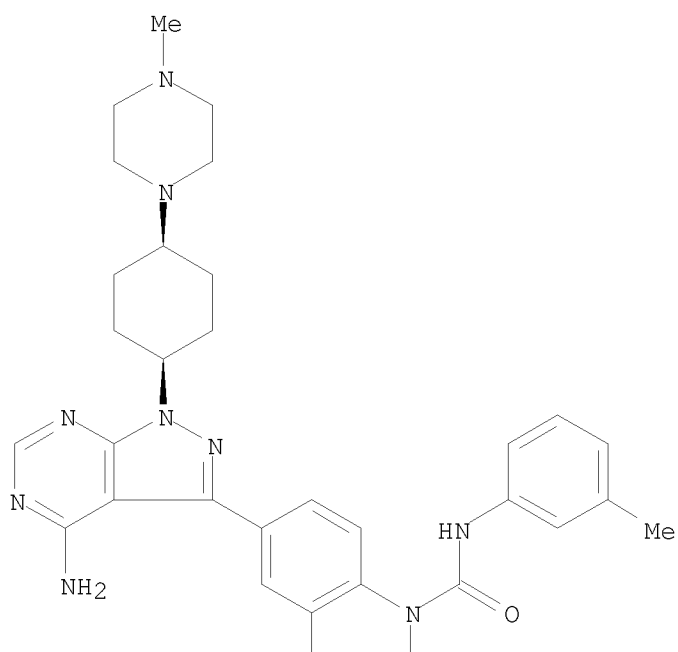
PAGE 2-A

F

RN 330788-52-8 CAPLUS
CN Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N-ethyl-N'-(3-methylphenyl)-
(CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

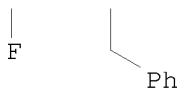
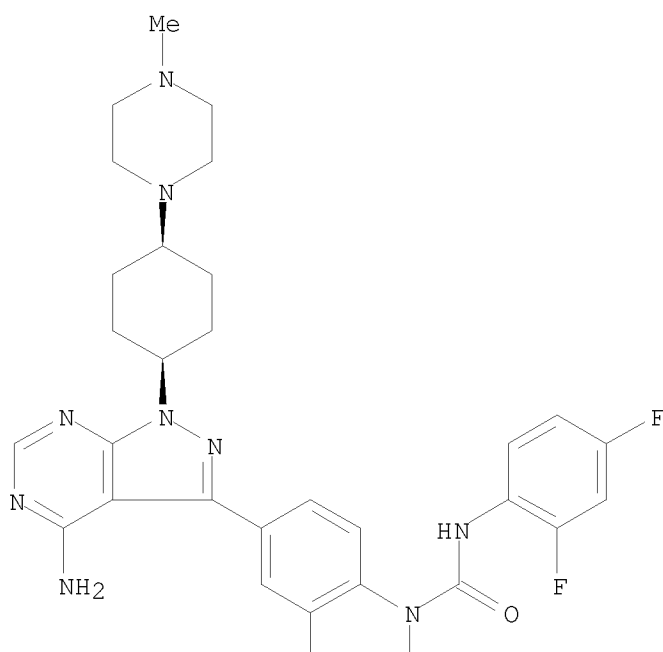


PAGE 2-A



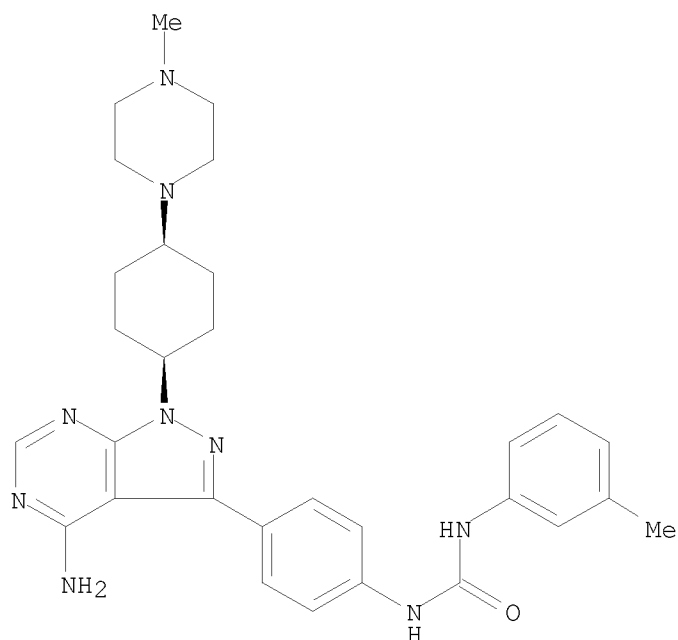
RN 330788-53-9 CAPLUS
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Relative stereochemistry.

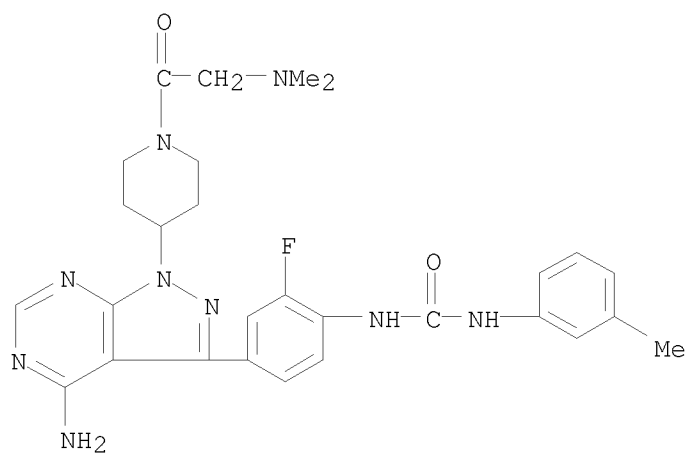


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CN	Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)	

Relative stereochemistry.



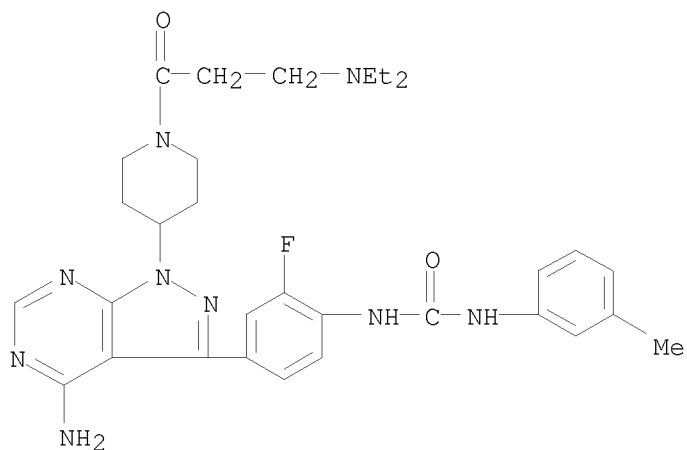
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 CN Urea, N-[4-[4-amino-1-[1-[2-(dimethylamino)acetyl]-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



RN 330788-57-3 CAPLUS
 CN Urea, N-[4-[4-amino-1-[1-[3-(diethylamino)-1-oxopropyl]-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, acetate (1:1) (CA INDEX NAME)

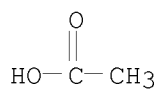
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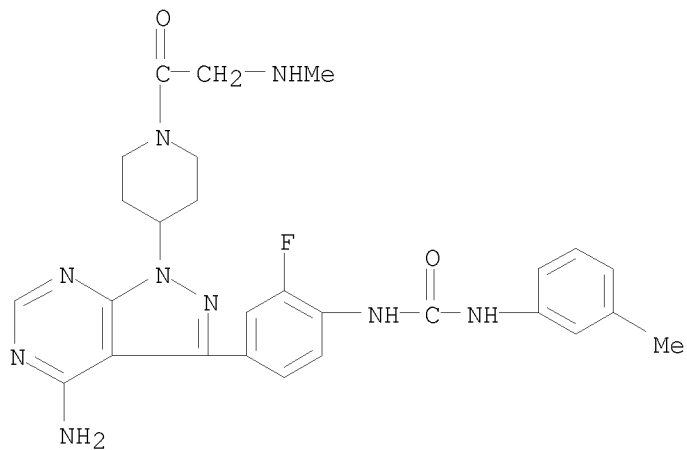


CM 2

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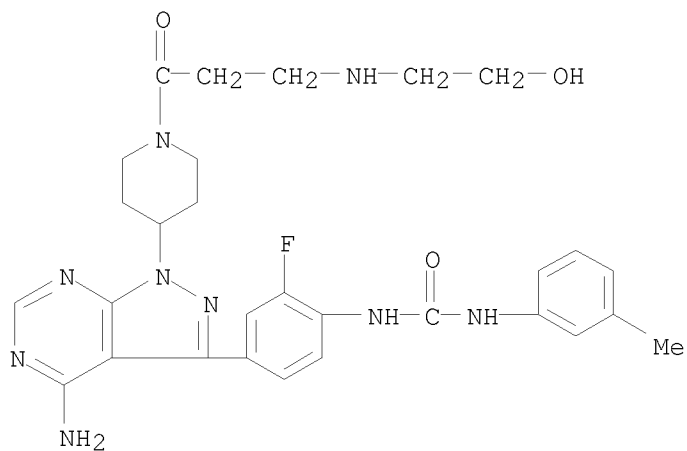
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RN 330788-60-8 CAPLUS
CN Urea, N-[4-[4-amino-1-[1-[3-[(2-hydroxyethyl)amino]-1-oxopropyl]-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, acetate (1:1) (CA INDEX NAME)

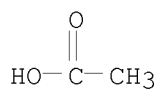
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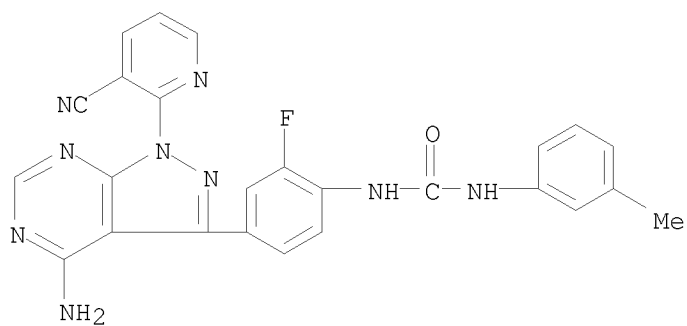


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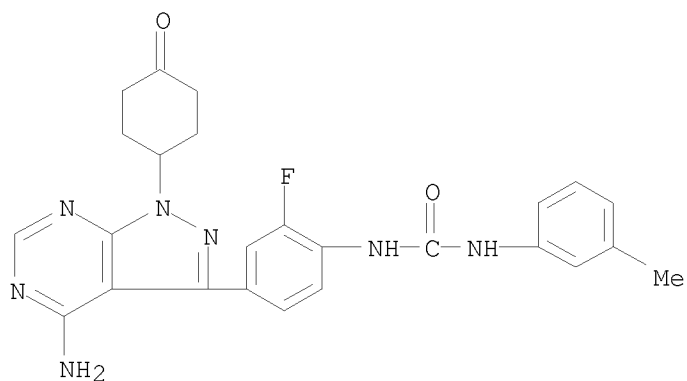
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CMF C2 H4 O2



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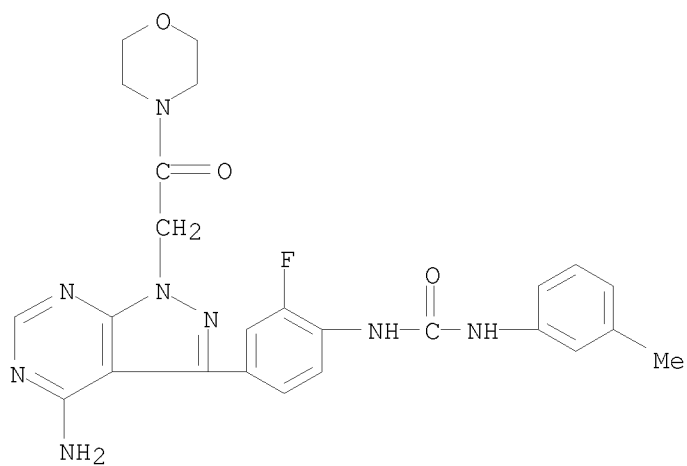


RN 330788-91-5 CAPLUS
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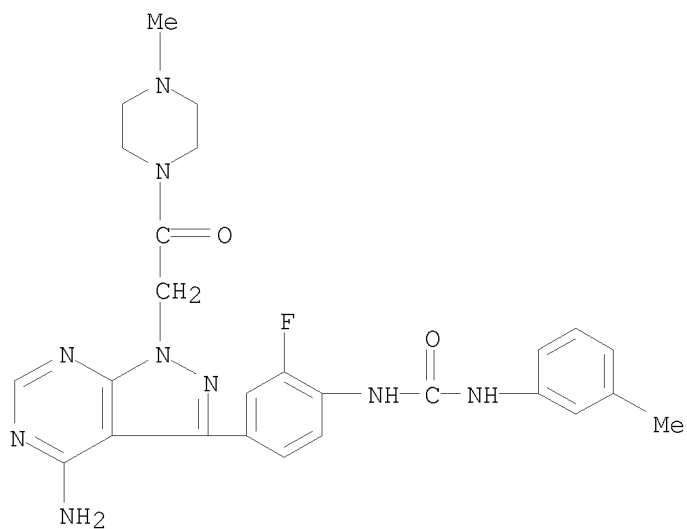
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CN Urea, N-[4-[4-amino-1-[2-(4-morpholinyl)-2-oxoethyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



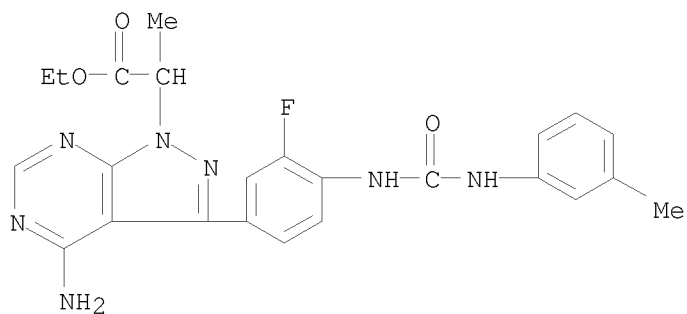
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CN Urea, N-[4-[4-amino-1-[2-(4-methyl-1-piperazinyl)-2-oxoethyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



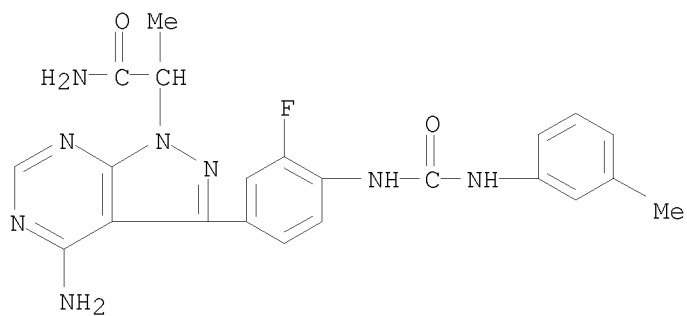
RN 330791-01-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-acetic acid, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-α-methyl-, ethyl ester
(CA INDEX NAME)



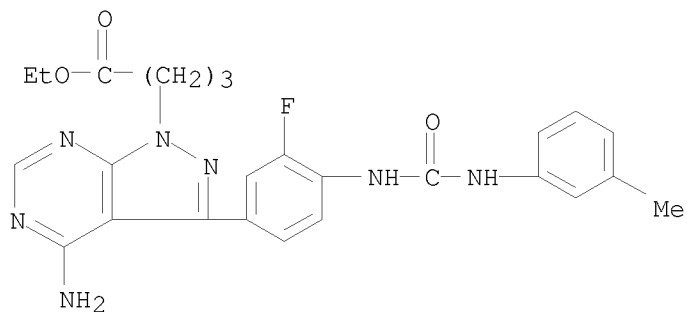
RN 330791-02-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-acetamide, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-α-methyl- (CA INDEX NAME)



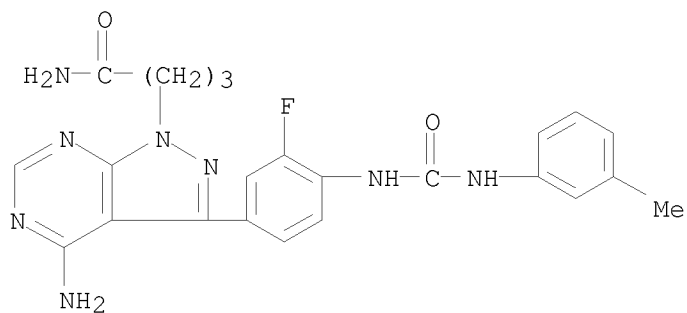
RN 330791-06-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-butanoic acid, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)



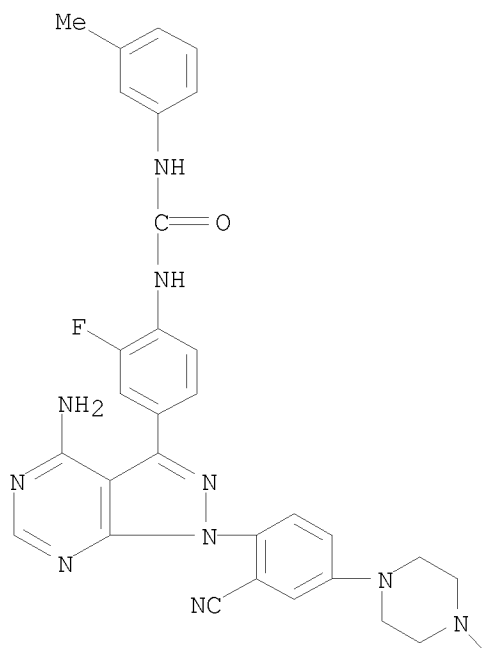
RN 330791-07-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-butanamide, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]- (CA INDEX NAME)



RN 330791-74-7 CAPLUS

CN Urea, N-[4-[4-amino-1-[2-cyano-4-(4-methyl-1-piperazinyl)phenyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:814851 CAPLUS

DOCUMENT NUMBER: 137:310930

TITLE: Preparation of 3-(azahetero)aryl-1H-pyrazolo[3,4-d]pyrimidin-3-amines as protein kinase inhibitors with antiangiogenic properties

INVENTOR(S): Hirst, Gavin C.; Rafferty, Paul; Ritter, Kurt; Calderwood, David; Wishart, Neil; Arnold, Lee D.; Friedman, Michael M.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: U.S. Pat. Appl. Publ., 426 pp., Cont.-in-part of U.S. Ser. No. 663,780.

CODEN: USXXCO

DOCUMENT TYPE: Patent

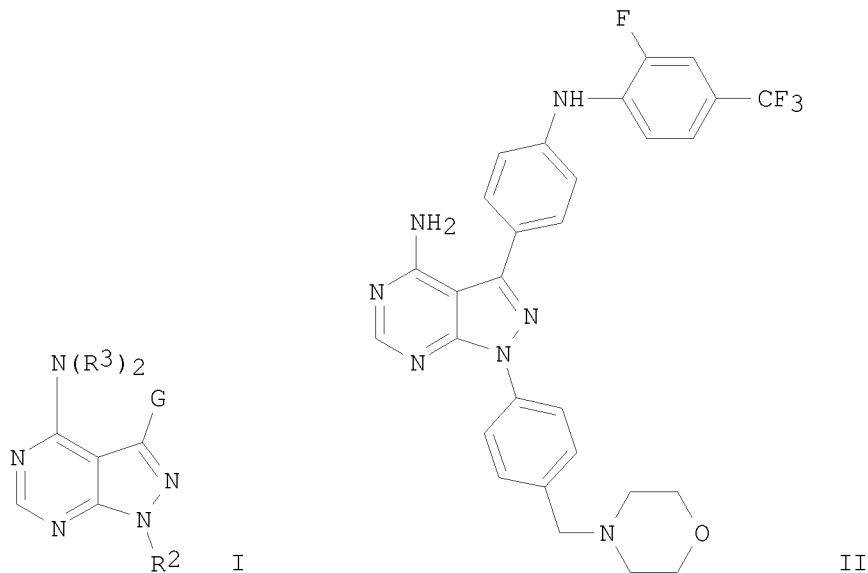
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

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US 20020156081	A1	20021024	US 2001-815310	20010322

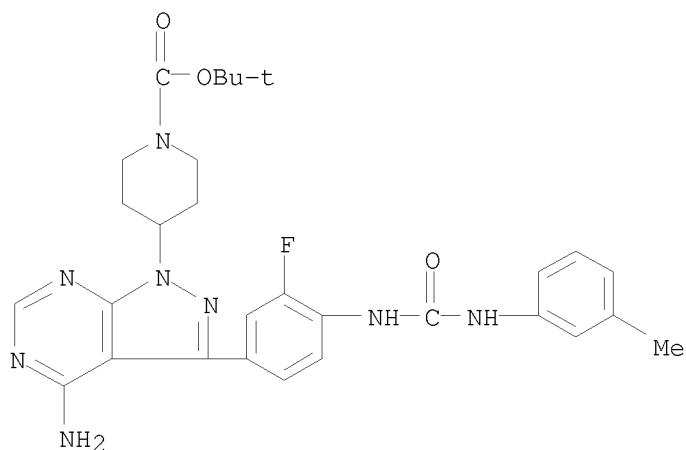
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US 6660744	B1	20031209	US 2000-663780	20000915
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WO 2002080926	A1	20021017	WO 2002-US9104	20020322
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EP 1385524	A1	20040204	EP 2002-746301	20020322
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CN 1520298	A	20040811	CN 2002-810250	20020322
JP 2004531513	T	20041014	JP 2002-578965	20020322
BR 2002005889	A	20041109	BR 2002-5889	20020322
ZA 2003006886	A	20040716	ZA 2003-6886	20030903
NO 2003004176	A	20031121	NO 2003-4176	20030919
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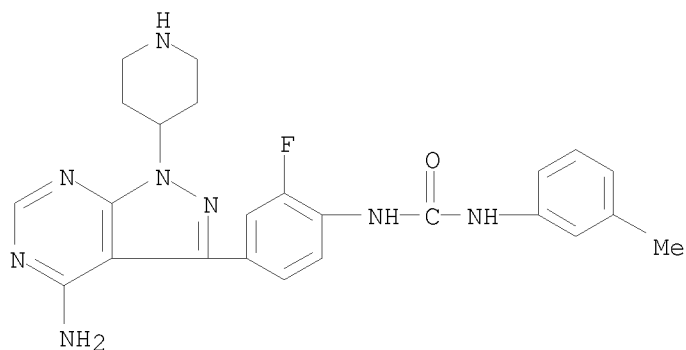
AB Title compds. I [wherein G = (un)substituted 5-6 membered (azahetero)aryl; R2 = H or (un)substituted trityl, cycloalkenyl, azaheteroaryl, or C6H4-4-CH2E; E = (un)substituted alkyl-OR, alkyl-CO2R, alkylheteroaryl, alkylheterocycloalkyl, or alkyl-NR2; R = independently H or

(un)substituted (cyclo)alkyl, or aryl(alkyl); R3 = independently H, OH, or (un)substituted alkyl, alkyl-CO, (hetero)aryl-CO, or alkoxy; or racemic diastereomeric mixts., optical isomers, pharmaceutically acceptable salts, prodrugs, and/or biol. active metabolites thereof] were prepared For example, 3-iodo-1H-pyrazolo[3,4-d]pyrimidin-4-amine was coupled with 4-fluorobenzaldehyde in the presence of NaH in DMF to give 4-(4-amino-3-iodo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)benzaldehyde. Treatment of the 3-iodopyrazolopyrimidine with N-[2-methoxy-4-(4,4,5,5,-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-2-fluoro-4-(trifluoromethyl)benzamide, Pd(PPh3)4, and Na2CO3 in H2O afforded the N-[4-(pyrazolopyrimidin-3-yl)phenyl]benzamide. Addition of morpholine to the benzaldehyde in the presence of Na(AcO)3BH in dichloroethane produced II. All exemplified compds. significantly inhibited either FGFR, PDGFR, KDR, Tie-2, Lck, Fyn, Blk, Lyn, or Src at concentration of $\leq 50 \mu\text{M}$. Certain compds. of the invention also significantly inhibited cdc2 or cellular VEGF-induced KDR tyrosine kinase phosphorylation at concns. of $\leq 50 \mu\text{M}$. Thus, I are useful for the treatment of a wide variety of disease states ameliorated by the inhibition of protein tyrosine kinase activity essential for angiogenic processes (no data).

- IT 330793-24-3P 330793-25-4P, N-[4-[4-Amino-1-(4-piperidyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea dihydrochloride 471925-82-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of [(hetero)aryl]pyrazolo[3,4-d]pyrimidinamines as protein kinase inhibitors with antiangiogenic properties)
- RN 330793-24-3 CAPLUS
- CN 1-Piperidinecarboxylic acid, 4-[4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



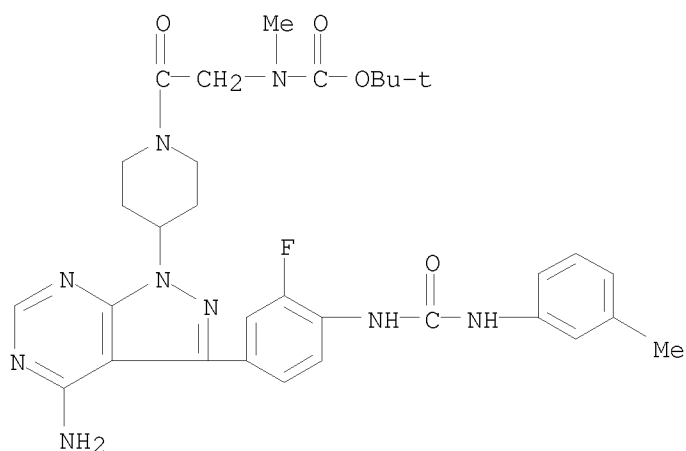
- RN 330793-25-4 CAPLUS
- CN Urea, N-[4-[4-amino-1-(4-piperidyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

RN 471925-82-3 CAPLUS

CN Carbamic acid, [2-[4-[4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-1-piperidinyl]-2-oxoethyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

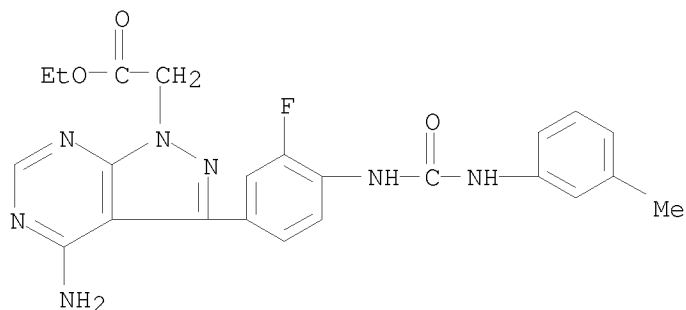


IT 471926-42-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(protein kinase inhibitor; preparation of [(hetero)aryl]pyrazolo[3,4-d]pyrimidinamines as protein kinase inhibitors with antiangiogenic properties)

RN 471926-42-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-acetic acid, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)



IT 330788-46-0P, cis-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(2,4-difluorophenyl)urea 330788-47-1P, trans-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methoxyphenyl)urea 330788-48-2P, trans-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methoxyphenyl)urea monoacetate 330788-50-6P, trans-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea monoacetate 330788-51-7P, cis-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea 330788-52-8P, cis-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N-ethyl-N'-(3-methylphenyl)urea 330788-53-9P, cis-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N-benzyl-N'-(2,4-difluorophenyl)urea 330788-54-0P, cis-N-[4-[4-Amino-1-[4-(4-methylpiperazino)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-(3-methylphenyl)urea 330788-55-1P, N-[4-[4-Amino-1-[1-[2-(dimethylamino)acetyl]-4-piperidyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea 330788-57-3P, N-[4-[4-Amino-1-[1-[3-(diethylamino)propanoyl]-4-piperidyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea monoacetate 330788-58-4P, N-[4-[4-Amino-1-[1-[2-(methylamino)acetyl]-4-piperidyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea 330788-60-8P, N-[4-[4-Amino-1-[1-[3-[(2-hydroxyethyl)amino]propanoyl]-4-piperidyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea monoacetate 330788-70-0P 330788-91-5P, N-[4-[4-Amino-1-(4-oxocyclohexyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea 330790-96-0P, N-[4-[4-Amino-1-(2-morpholino-2-oxoethyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea 330790-97-1P, N-[4-[4-Amino-1-[2-(4-methylpiperazino)-2-oxoethyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea 330791-01-0P 330791-02-1P 330791-06-5P 330791-07-6P 330791-74-7P, N-[4-[4-Amino-1-[2-cyano-4-(4-methylpiperazino)phenyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)urea

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(protein kinase inhibitor; preparation of [(hetero)aryl]pyrazolo[3,4-d]pyrimidinamines as protein kinase inhibitors with antiangiogenic properties)

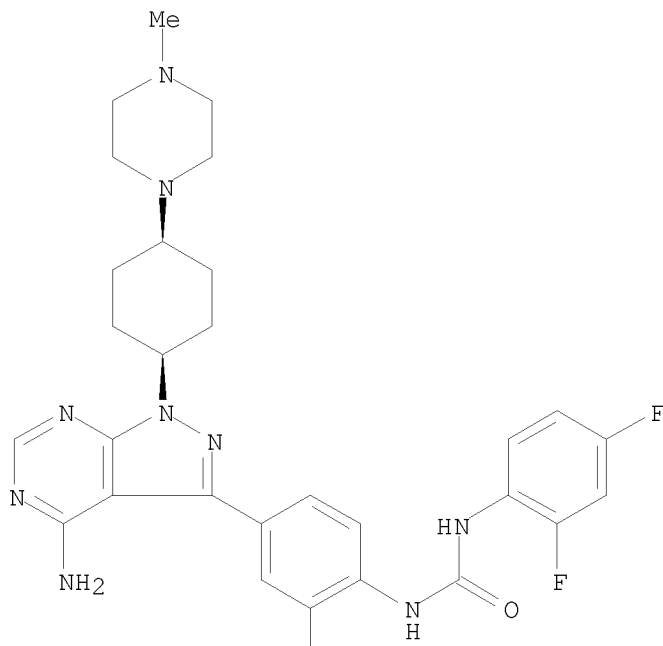
RN 330788-46-0 CAPLUS

CN Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-

pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(2,4-difluorophenyl)-
(CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

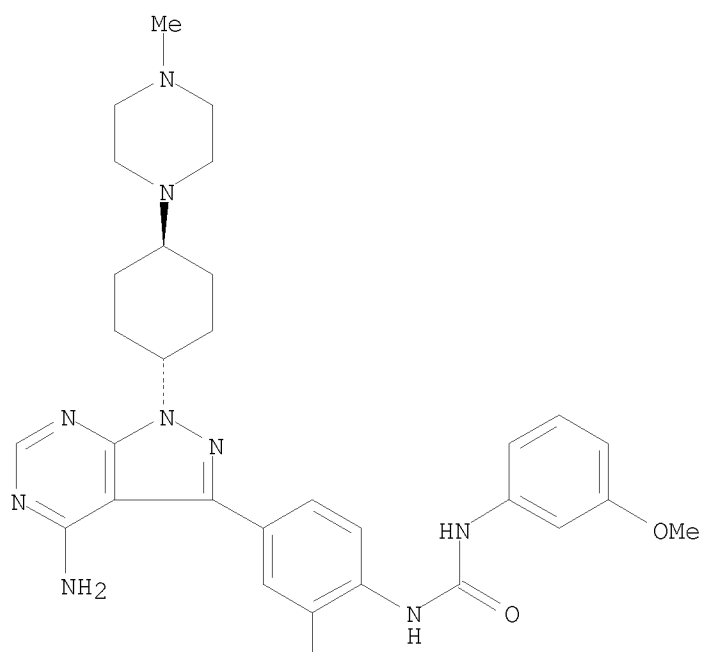


PAGE 2-A



RN 330788-47-1 CAPLUS
CN Urea, N-[4-[4-amino-1-[trans-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methoxyphenyl)- (CA INDEX NAME)

Relative stereochemistry.



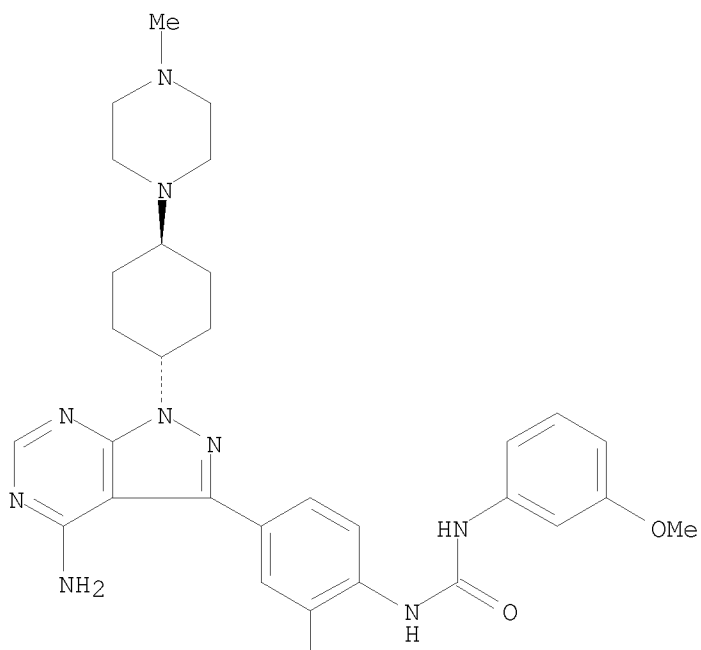
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F

RN 330788-48-2 CAPLUS
 CN Urea, N-[4-[4-amino-1-[trans-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methoxyphenyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

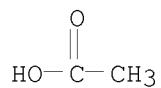
CRN 330788-47-1
 CMF C30 H36 F N9 O2

Relative stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2



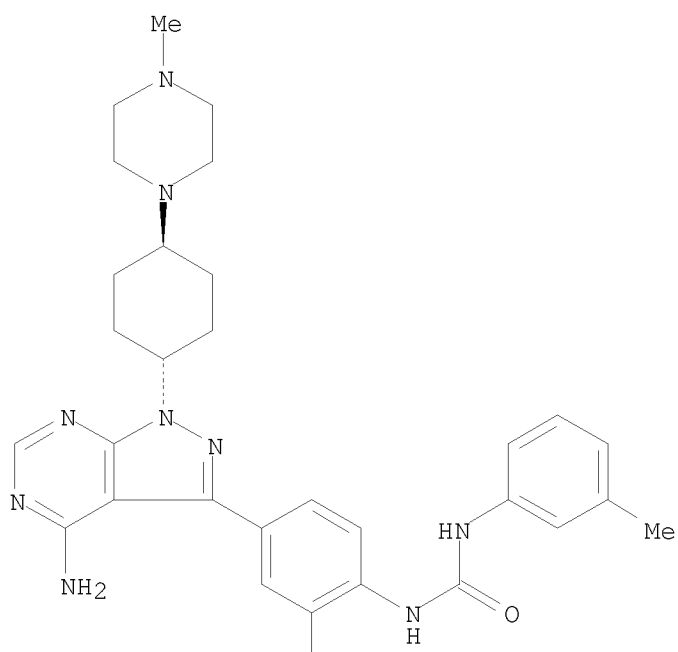
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CN	Urea, N-[4-[4-amino-1-[trans-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, acetate (1:1) (CA INDEX NAME)	

CM 1

CRN 330788-49-3
CMF C30 H36 F N9 O

Relative stereochemistry.

PAGE 1-A

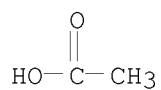


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CM 2

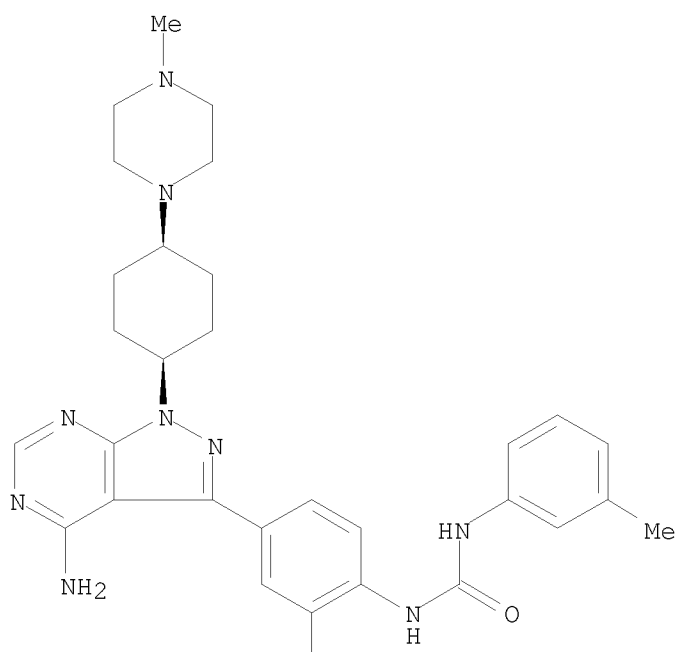
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RN 330788-51-7 CAPLUS
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Relative stereochemistry.

PAGE 1-A



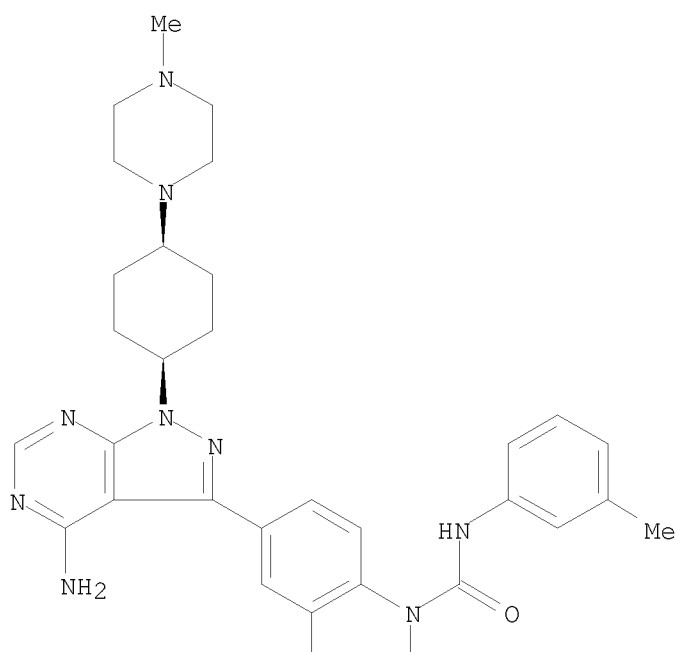
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RN 330788-52-8 CAPLUS
CN Urea, N-[4-[4-amino-1-[cis-4-(4-methyl-1-piperazinyl)cyclohexyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N-ethyl-N'-(3-methylphenyl)-
(CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



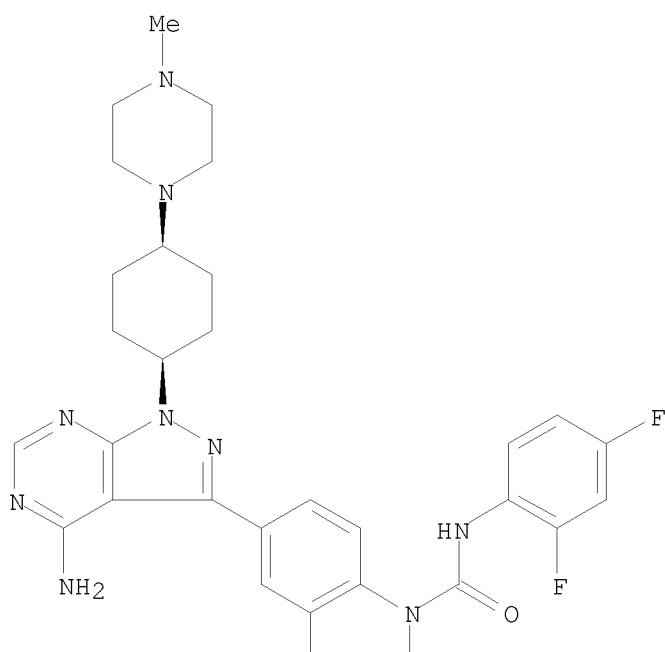
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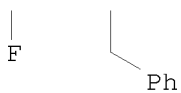
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Relative stereochemistry.

PAGE 1-A

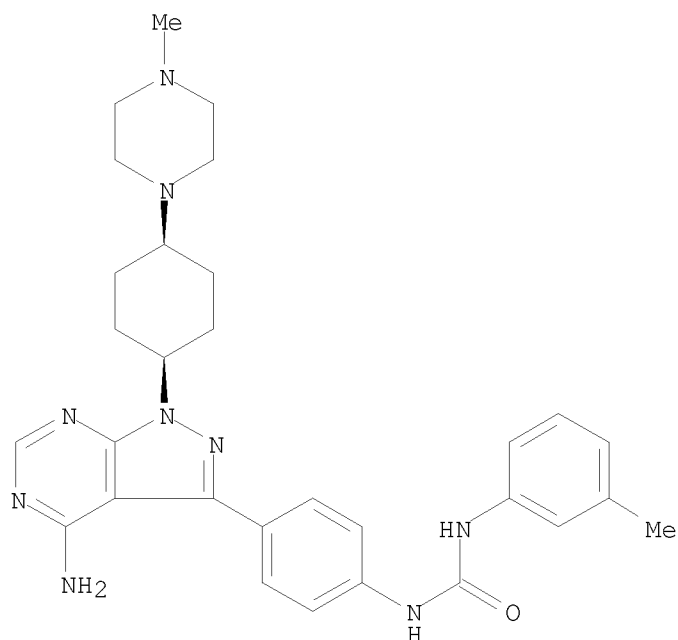


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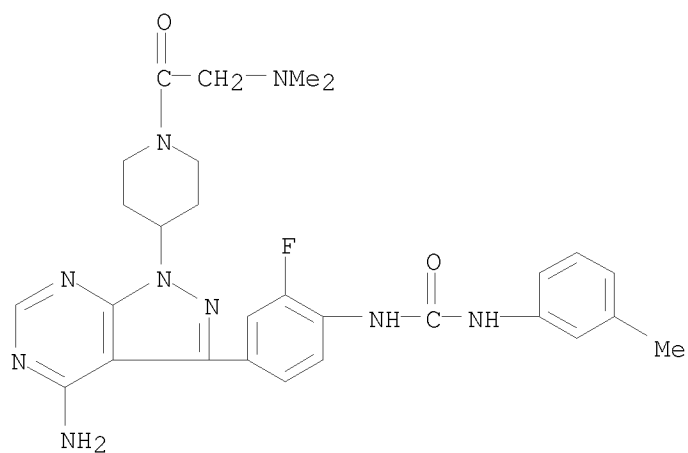


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Relative stereochemistry.



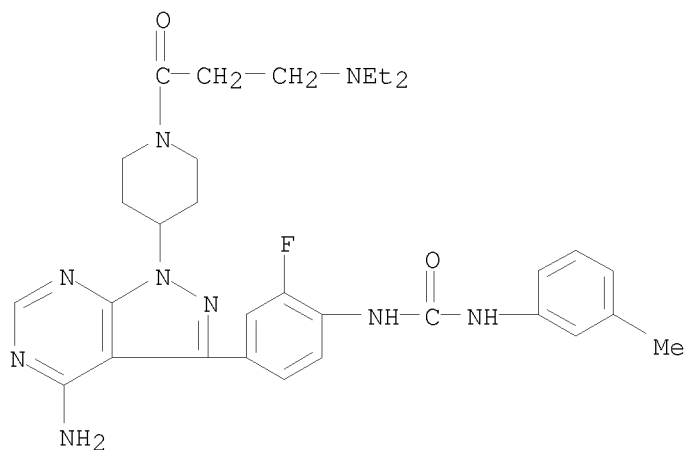
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RN 330788-57-3 CAPLUS
 CN Urea, N-[4-[4-amino-1-[1-[3-(diethylamino)-1-oxopropyl]-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, acetate (1:1) (CA INDEX NAME)

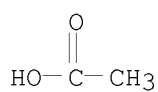
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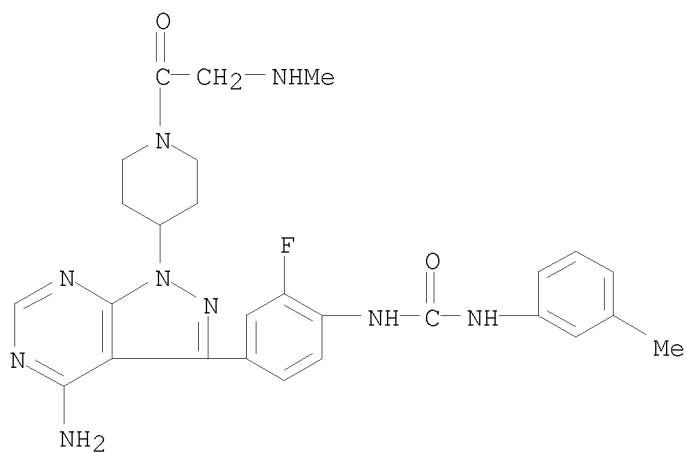


CM 2

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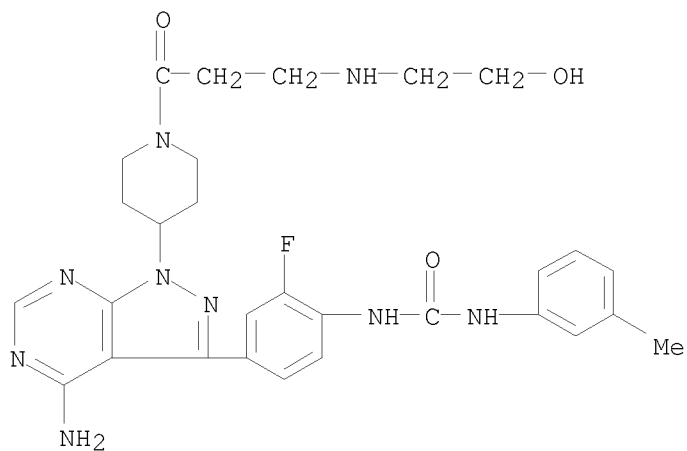
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CN Urea, N-[4-[4-amino-1-[1-[2-(methylamino)acetyl]-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



RN 330788-60-8 CAPLUS
CN Urea, N-[4-[4-amino-1-[1-[3-[(2-hydroxyethyl)amino]-1-oxopropyl]-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)-, acetate (1:1) (CA INDEX NAME)

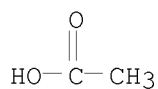
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CRN 330788-59-5
CMF C29 H34 F N9 O3

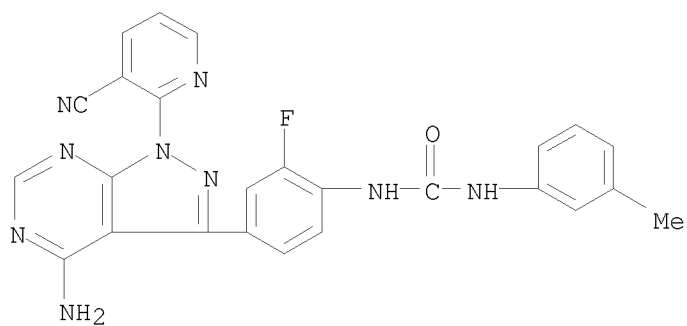


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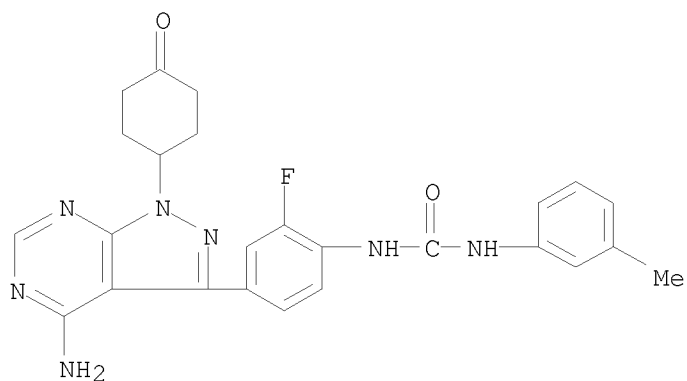
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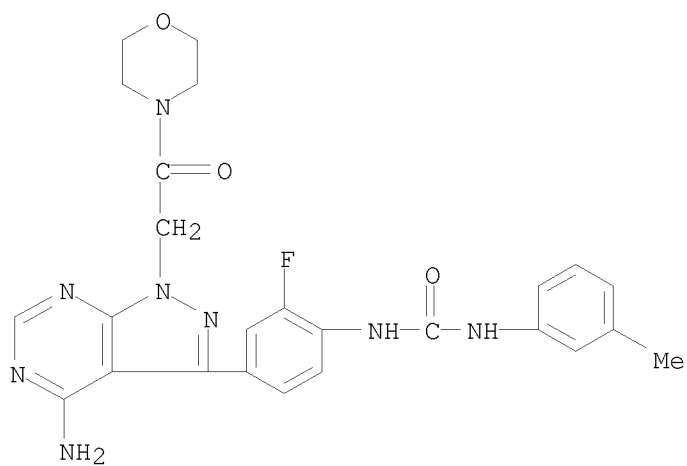


RN 330788-91-5 CAPLUS
CN Urea, N-[4-[4-amino-1-(4-oxocyclohexyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



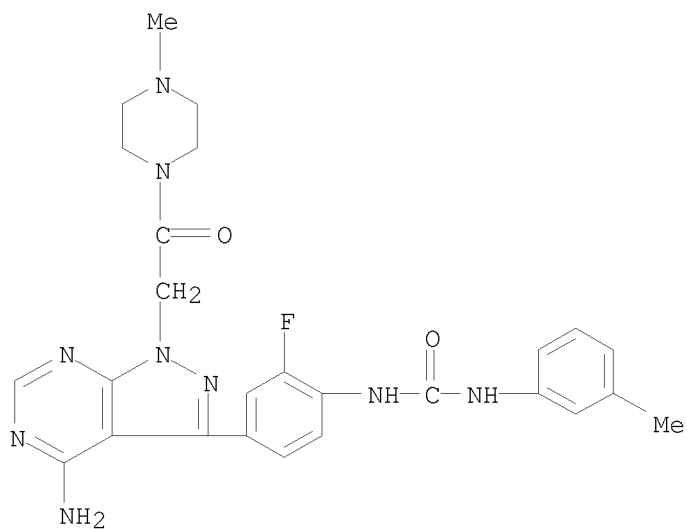
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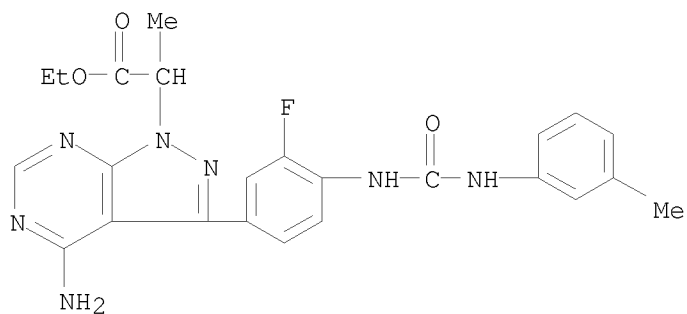
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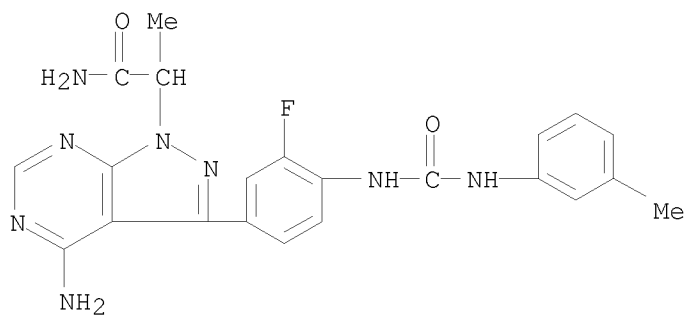
RN 330791-01-0 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-acetic acid, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-α-methyl-, ethyl ester
(CA INDEX NAME)



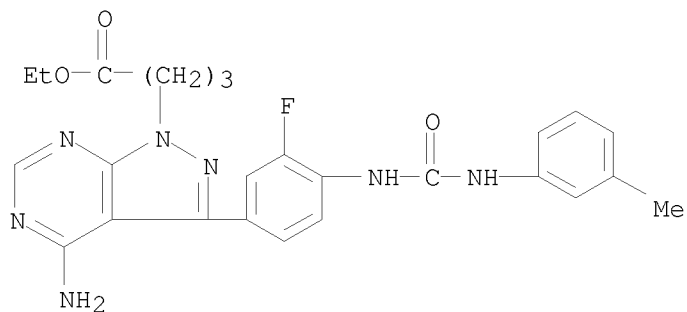
RN 330791-02-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-acetamide, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-α-methyl- (CA INDEX NAME)



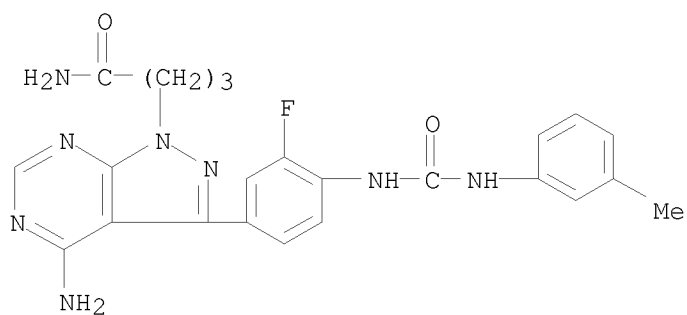
RN 330791-06-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-butanoic acid, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)



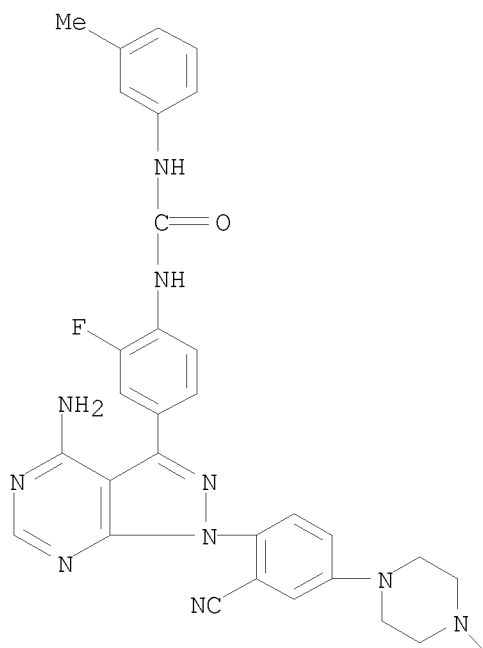
RN 330791-07-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-1-butanamide, 4-amino-3-[3-fluoro-4-[[[(3-methylphenyl)amino]carbonyl]amino]phenyl]- (CA INDEX NAME)



RN 330791-74-7 CAPLUS

CN Urea, N-[4-[4-amino-1-[2-cyano-4-(4-methyl-1-piperazinyl)phenyl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-(3-methylphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 115 THERE ARE 115 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

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L4 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:282531 CAPLUS

DOCUMENT NUMBER: 138:321286

TITLE: Preparation of pyrazolo[3,4-d]pyrimidine derivatives for treating diseases associated with inappropriate angiogenesis

INVENTOR(S): Adams, Jerry Leroy; Kaspavec, Jiri; Silva, Domingos; Yuan, Catherine C. K.

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 108 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003029209	A2	20030410	WO 2002-US31293	20021001
WO 2003029209	A3	20040212		

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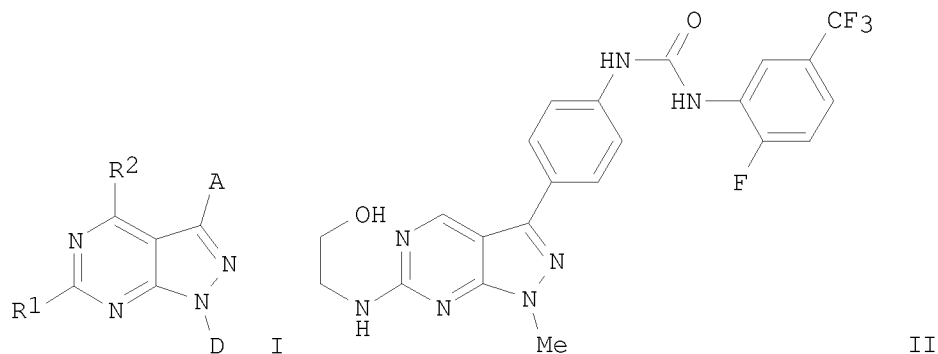
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JP 2005504828 T 20050217 JP 2003-532459 20021001
AT 403657 T 20080815 AT 2002-776075 20021001
US 20040198751 A1 20041007 US 2004-491711 20040402
US 7217710 B2 20070515
US 20070293489 A1 20071220 US 2007-747274 20070511

PRIORITY APPLN. INFO.: US 2001-326506P P 20011002
WO 2002-US31293 W 20021001
US 2004-491711 A1 20040402

OTHER SOURCE(S): MARPAT 138:321286
GI



AB The title compds. [I; A = (hetero)aryl substituted with at least one NHCOR₈, NHSO₂R₉ or NHCSR₈; D = H, alkyl, aryl, etc.; R₁ = NR₇R₇, NR₇(R₁₀NR₁₂R₁₃); R₂ = H, NR₇R₇, :NH; R₇ = H, alkyl, aryl, etc.; R₈ = NR₁₂R₁₃, NR₇(R₁₀NR₁₂R₁₃); R₉ = (un)substituted (hetero)aryl; R₁₀ = alkylene; R₁₂ = H, alkyl, aryl, etc.; R₁₃ = H, alkyl, aryl, etc.], useful for inhibiting TIE-2 kinase, VEGFR-2 kinase and/or VEGFR-3 kinase, were prepared Thus, reacting 2-[3-(4-aminophenyl)-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-6-ylamino]ethanol (preparation given) with 2-fluoro-5-trifluoromethylphenyl isocyanate in N-methylpyrrolidine afforded II which showed IC₅₀ of ≥ 100 to < 300 nM in TIE2-FP assay.

IT 508222-38-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrazolo[3,4-d]pyrimidine derivs. for treating diseases associated with inappropriate angiogenesis)

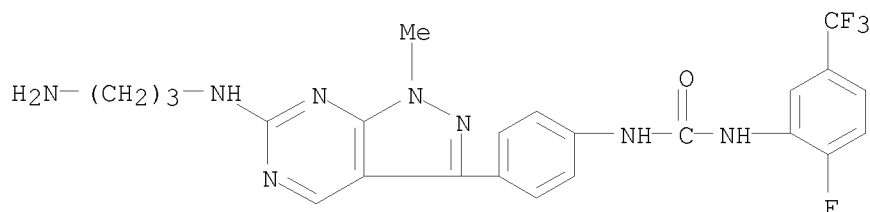
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2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

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CRN 508222-37-5

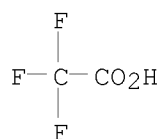
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CM 2

CRN 76-05-1

CMF C2 H F3 O2



IT 508221-22-5P 508221-23-6P 508221-25-8P
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508223-51-6P 508223-52-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(preparation of pyrazolo[3,4-d]pyrimidine derivs. for treating diseases
associated with inappropriate angiogenesis)

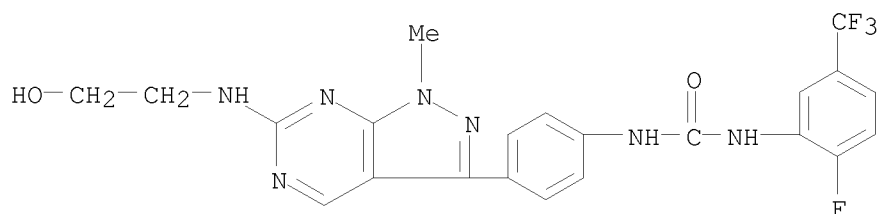
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CM 1

CRN 508221-21-4

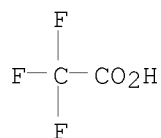
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CM 2

CRN 76-05-1

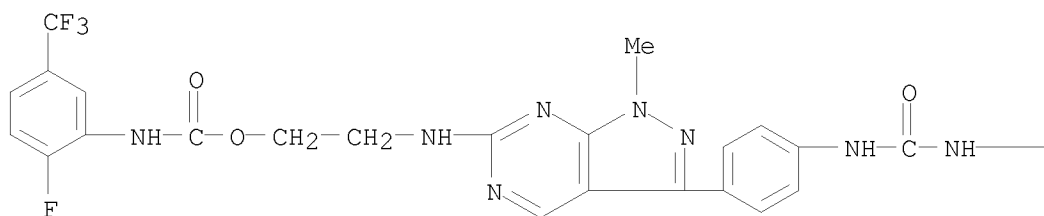
CMF C2 H F3 O2



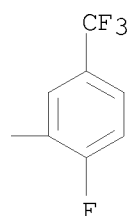
RN 508221-23-6 CAPLUS

CN Carbamic acid, [2-fluoro-5-(trifluoromethyl)phenyl]-, 2-[[3-[4-[[[2-fluoro-5-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]amino]ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



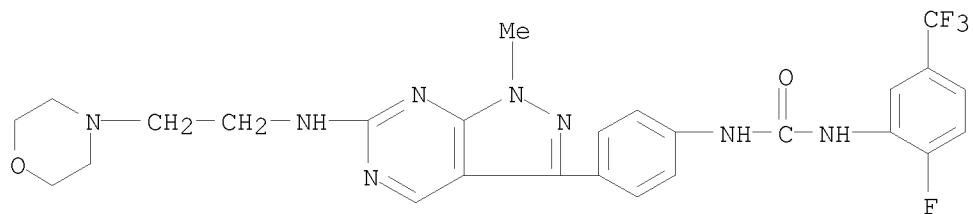
PAGE 1-B



RN 508221-25-8 CAPLUS
 CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

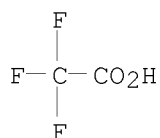
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CM 2

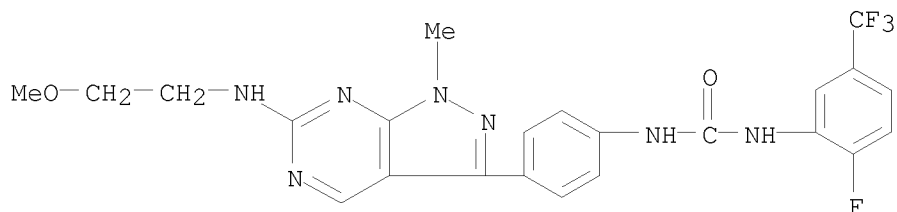
CRN 76-05-1
 CMF C2 H F3 O2



RN 508221-27-0 CAPLUS
 CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[6-[(2-methoxyethyl)amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

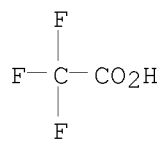
CM 1

CRN 508221-26-9
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CM 2

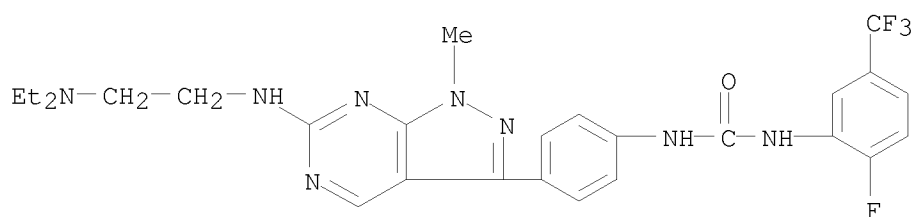
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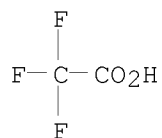
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CM 2

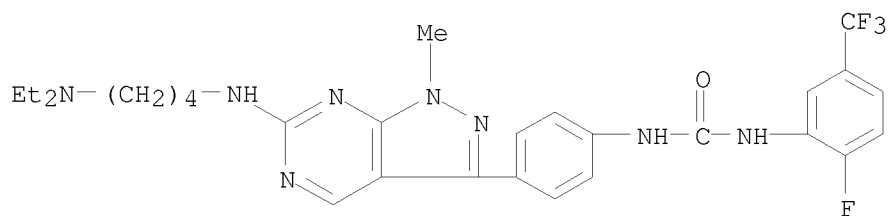
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RN 508221-31-6 CAPLUS
 CN Urea, N-[4-[6-[[4-(diethylamino)butyl]amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

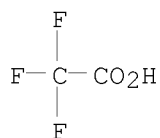
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CM 2

CRN 76-05-1

CMF C2 H F3 O2



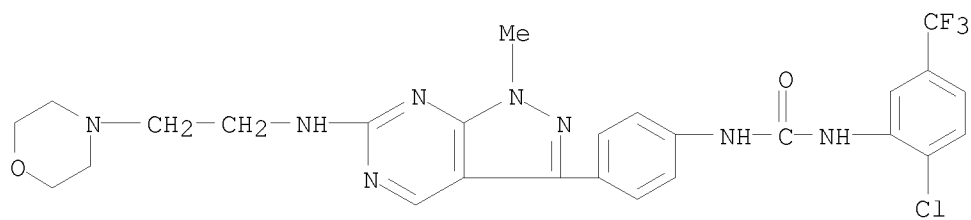
RN 508221-35-0 CAPLUS

CN Urea, N-[2-chloro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-34-9

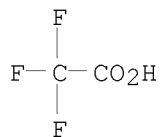
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CM 2

CRN 76-05-1

CMF C2 H F3 O2



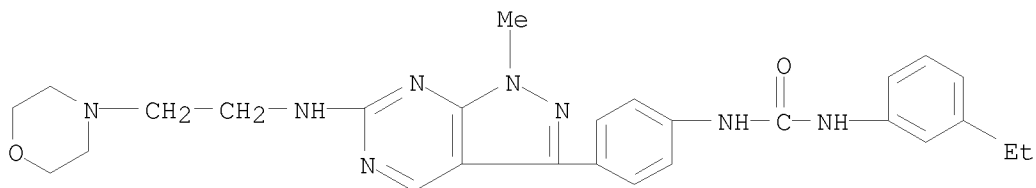
RN 508221-37-2 CAPLUS

CN Urea, N-(3-ethylphenyl)-N'-[4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-

1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1)
(CA INDEX NAME)

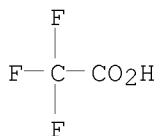
CM 1

CRN 508221-36-1
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CM 2

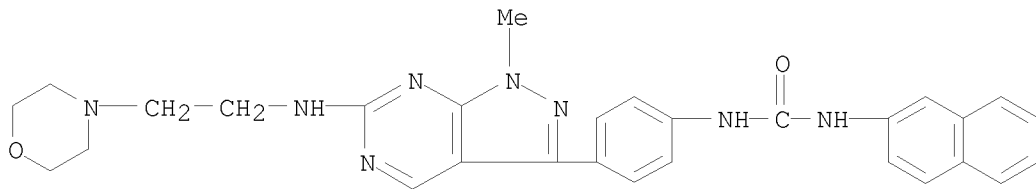
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RN 508221-39-4 CAPLUS
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(CA INDEX NAME)

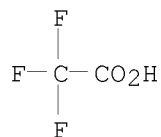
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CM 2

CRN 76-05-1
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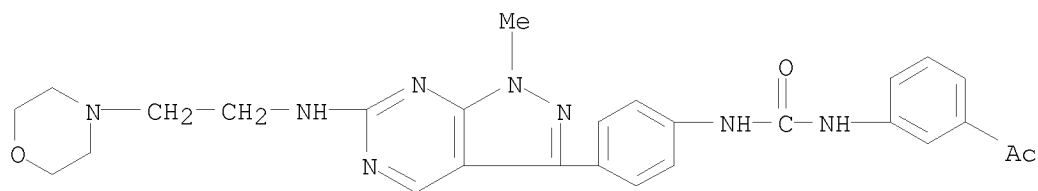
RN 508221-41-8 CAPLUS

CN Urea, N-(3-acetylphenyl)-N'-[4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1)
(CA INDEX NAME)

CM 1

CRN 508221-40-7

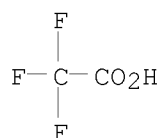
CMF C27 H30 N8 O3



CM 2

CRN 76-05-1

CMF C2 H F3 O2



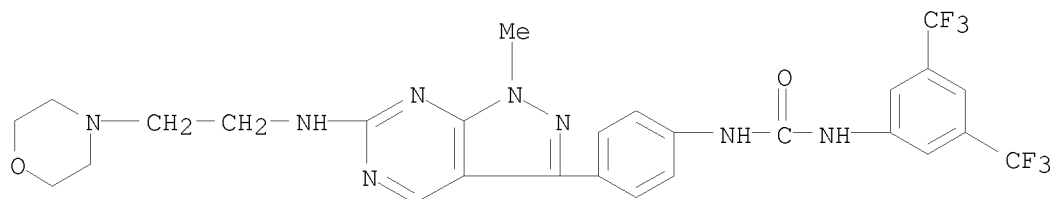
RN 508221-43-0 CAPLUS

CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-42-9

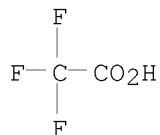
CMF C27 H26 F6 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



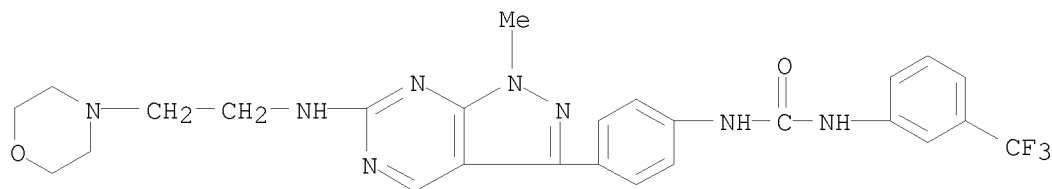
RN 508221-45-2 CAPLUS

CN Urea, N-[4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[3-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-44-1

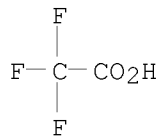
CMF C26 H27 F3 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



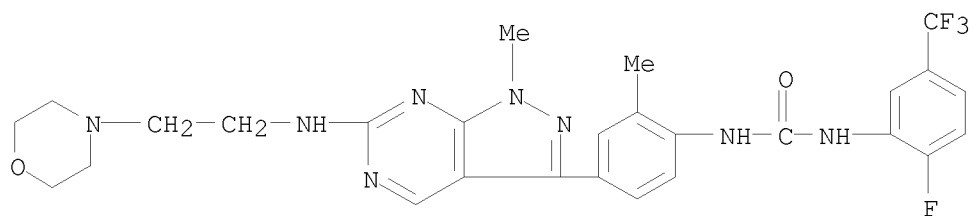
RN 508221-47-4 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[2-methyl-4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-46-3

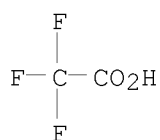
CMF C27 H28 F4 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



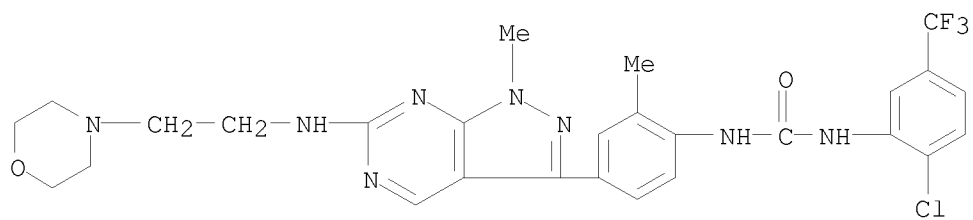
RN 508221-49-6 CAPLUS

CN Urea, N-[2-chloro-5-(trifluoromethyl)phenyl]-N'-[2-methyl-4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-48-5

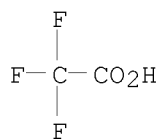
CMF C27 H28 Cl F3 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 508221-51-0 CAPLUS

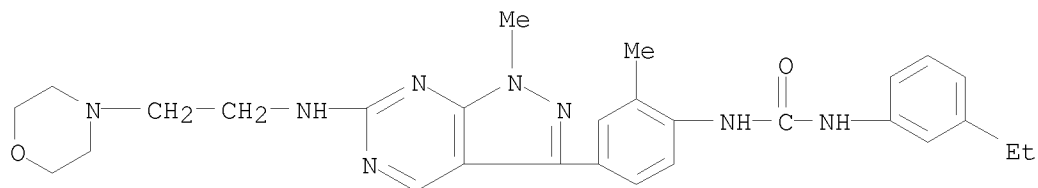
CN Urea, N-(3-ethylphenyl)-N'-[2-methyl-4-[1-methyl-6-[[2-(4-

morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-,
2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-50-9

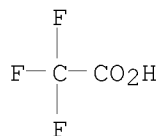
CMF C28 H34 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



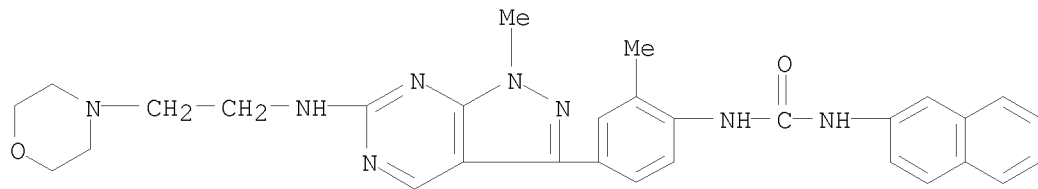
RN 508221-53-2 CAPLUS

CN Urea, N-[2-methyl-4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-2-naphthalenyl-,
2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-52-1

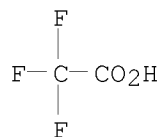
CMF C30 H32 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



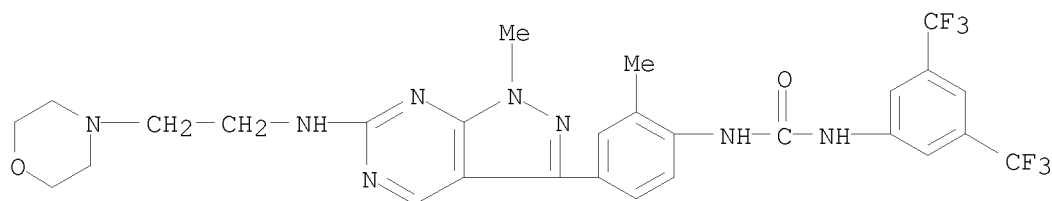
RN 508221-55-4 CAPLUS

CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[2-methyl-4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-54-3

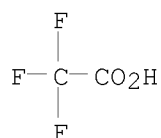
CMF C28 H28 F6 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



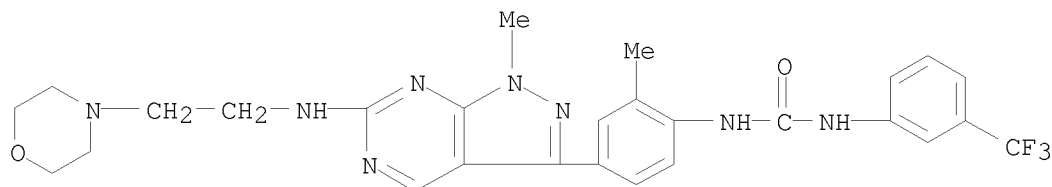
RN 508221-57-6 CAPLUS

CN Urea, N-[2-methyl-4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[3-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-56-5

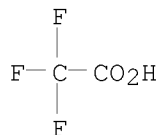
CMF C27 H29 F3 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



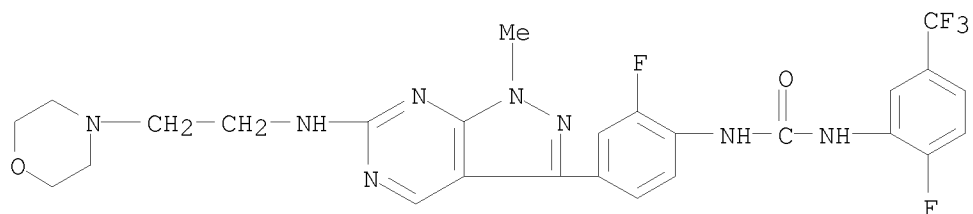
RN 508221-59-8 CAPLUS

CN Urea, N-[2-fluoro-4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-58-7

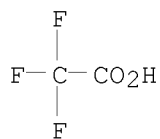
CMF C26 H25 F5 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



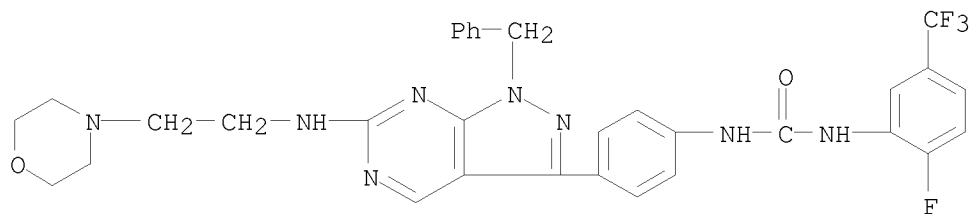
RN 508221-61-2 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[6-[[2-(4-morpholinyl)ethyl]amino]-1-(phenylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-60-1

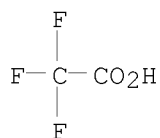
CMF C32 H30 F4 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



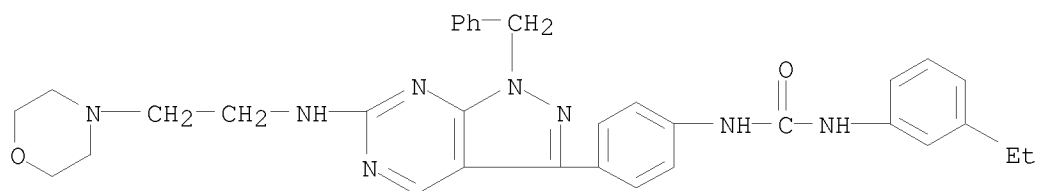
RN 508221-65-6 CAPLUS

CN Urea, N-(3-ethylphenyl)-N'-[4-[6-[[2-(4-morpholinyl)ethyl]amino]-1-(phenylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-64-5

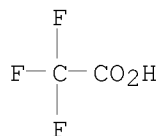
CMF C33 H36 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 508221-67-8 CAPLUS

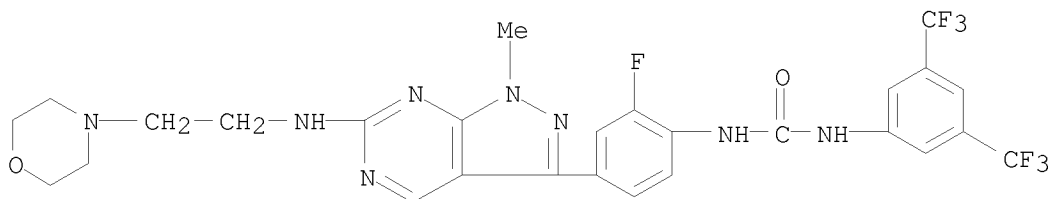
CN Urea, N-[3,5-bis(trifluoromethyl)phenyl]-N'-[2-fluoro-4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-,

2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-66-7

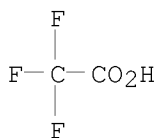
CMF C27 H25 F7 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



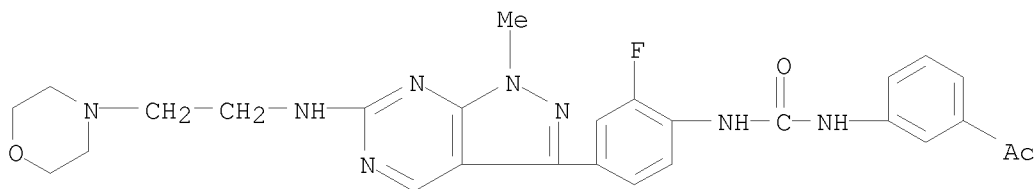
RN 508221-69-0 CAPLUS

CN Urea, N-(3-acetylphenyl)-N'-[2-fluoro-4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-68-9

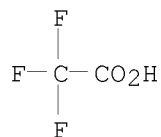
CMF C27 H29 F N8 O3



CM 2

CRN 76-05-1

CMF C2 H F3 O2



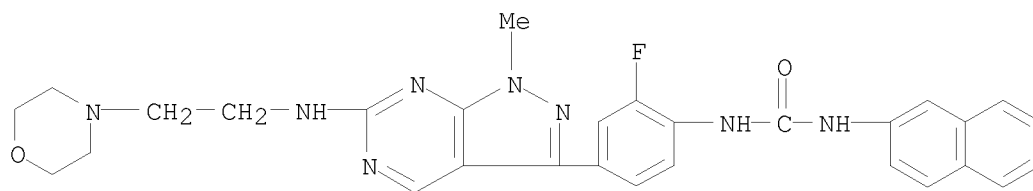
RN 508221-71-4 CAPLUS

CN Urea, N-[2-fluoro-4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-2-naphthalenyl-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-70-3

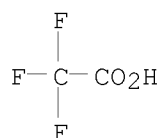
CMF C29 H29 F N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



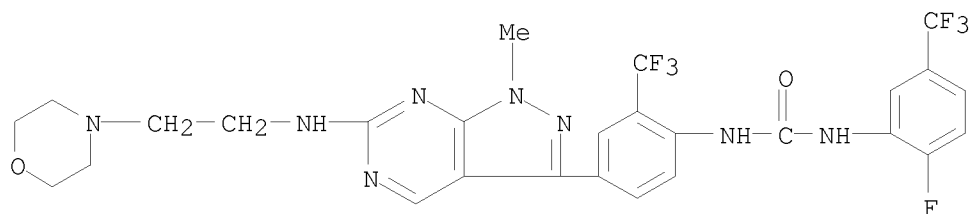
RN 508221-73-6 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-72-5

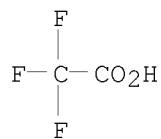
CMF C27 H25 F7 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



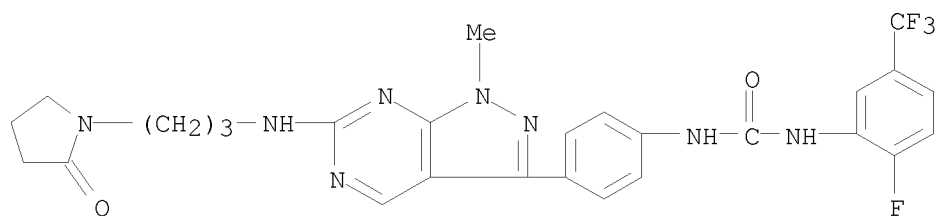
RN 508221-81-6 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-80-5

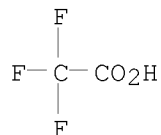
CMF C27 H26 F4 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



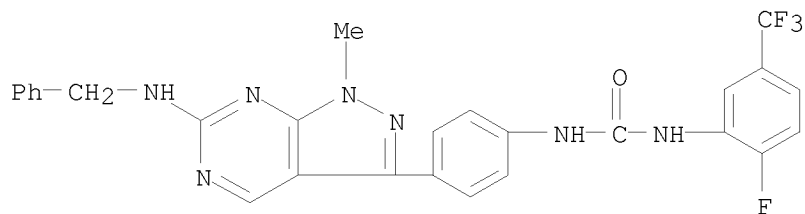
RN 508221-83-8 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[(phenylmethyl)amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-82-7

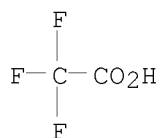
CMF C27 H21 F4 N7 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



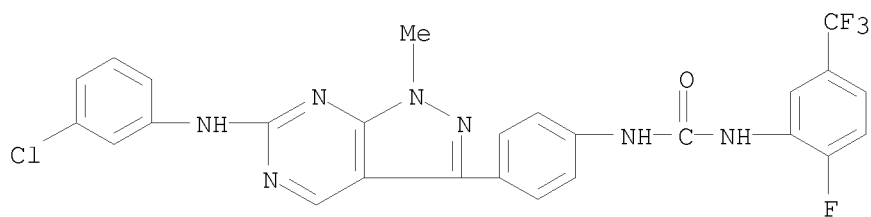
RN 508221-85-0 CAPLUS

CN Urea, N-[4-[6-[(3-chlorophenyl)amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-84-9

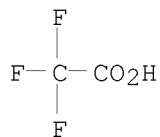
CMF C26 H18 Cl F4 N7 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 508221-87-2 CAPLUS

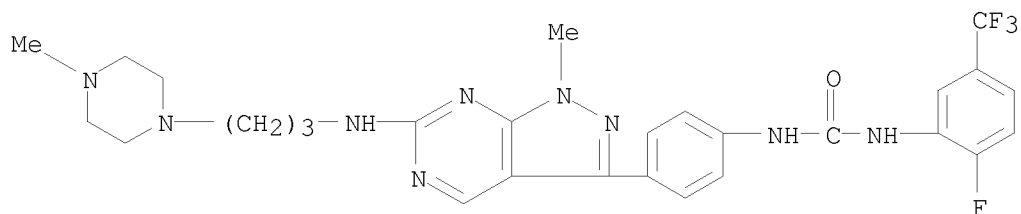
CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[3-(4-

methyl-1-piperaziny]propyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-86-1

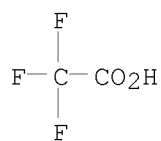
CMF C28 H31 F4 N9 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



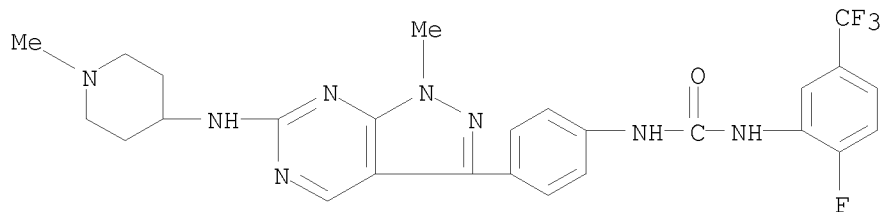
RN 508221-89-4 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[(1-methyl-4-piperidiny]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-88-3

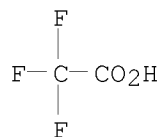
CMF C26 H26 F4 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



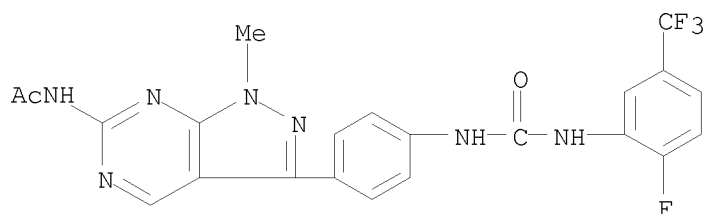
RN 508221-98-5 CAPLUS

CN Acetamide, N-[3-[4-[[[2-fluoro-5-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508221-97-4

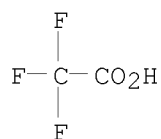
CMF C22 H17 F4 N7 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



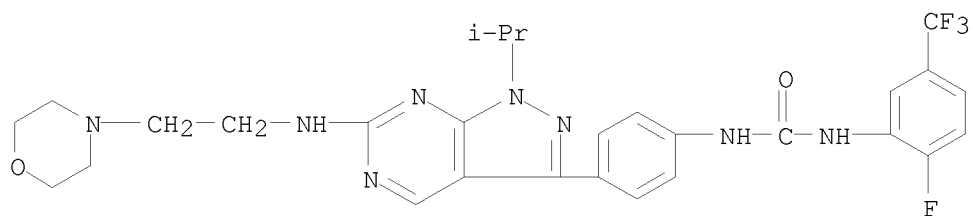
RN 508222-08-0 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-(1-methylethyl)-6-[[2-(4-morpholinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-07-9

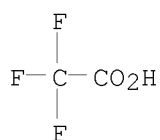
CMF C28 H30 F4 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



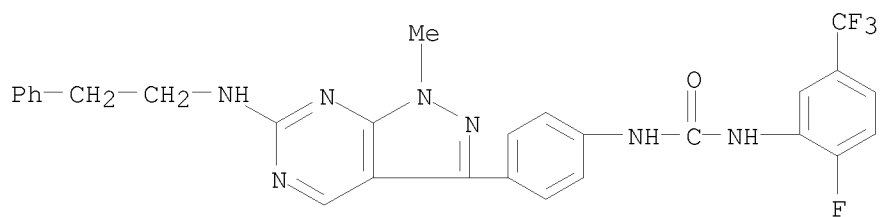
RN 508222-12-6 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[(2-phenylethyl)amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-11-5

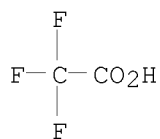
CMF C28 H23 F4 N7 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 508222-14-8 CAPLUS

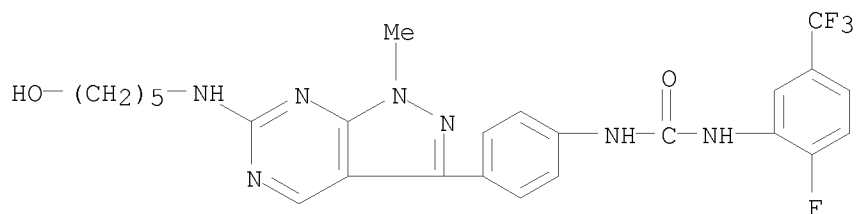
CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[6-[(5-

hydroxypentyl)amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-,
2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-13-7

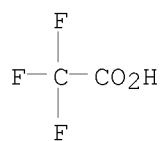
CMF C25 H25 F4 N7 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



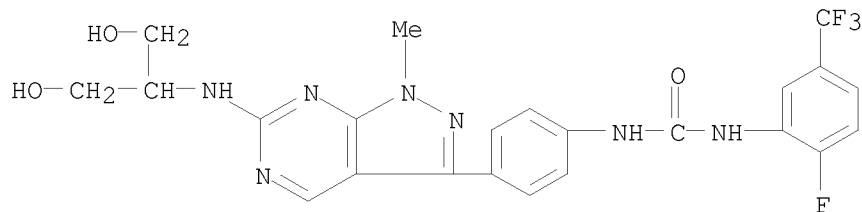
RN 508222-16-0 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[6-[2-hydroxy-1-(hydroxymethyl)ethyl]amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-15-9

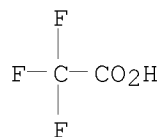
CMF C23 H21 F4 N7 O3



CM 2

CRN 76-05-1

CMF C2 H F3 O2



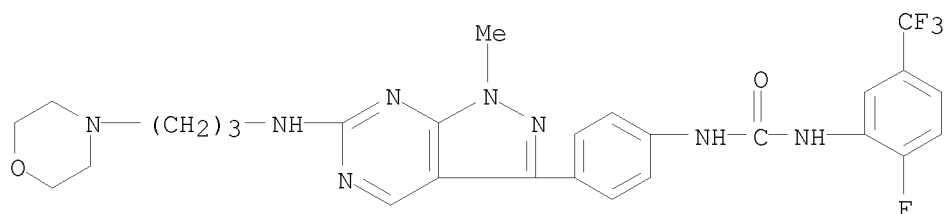
RN 508222-18-2 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[3-(4-morpholinyl)propyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-17-1

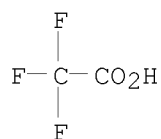
CMF C27 H28 F4 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



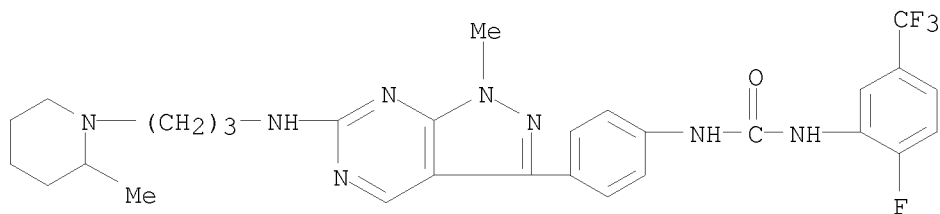
RN 508222-20-6 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[3-(2-methyl-1-piperidinyl)propyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-19-3

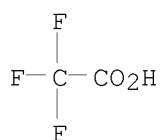
CMF C29 H32 F4 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



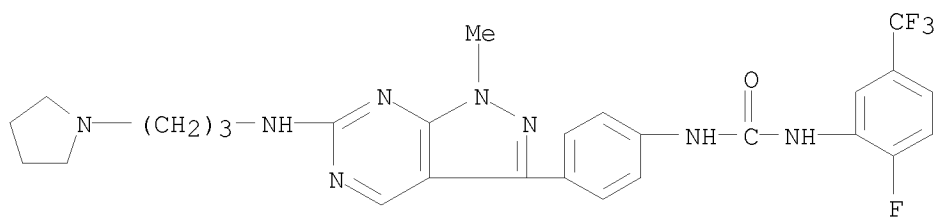
RN 508222-22-8 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[3-(1-pyrrolidinyl)propyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-21-7

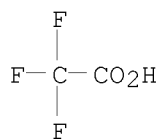
CMF C27 H28 F4 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 508222-24-0 CAPLUS

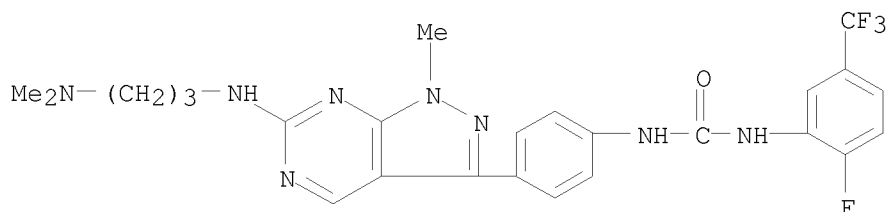
CN Urea, N-[4-[6-[[3-(dimethylamino)propyl]amino]-1-methyl-1H-pyrazolo[3,4-

d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-,
2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-23-9

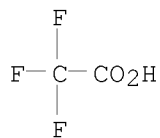
CMF C25 H26 F4 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



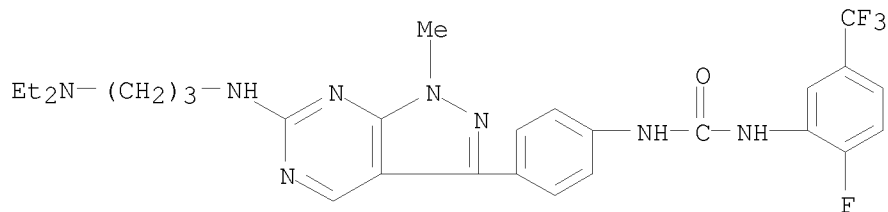
RN 508222-26-2 CAPLUS

CN Urea, N-[4-[6-[3-(diethylamino)propyl]amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-,
2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-25-1

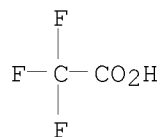
CMF C27 H30 F4 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



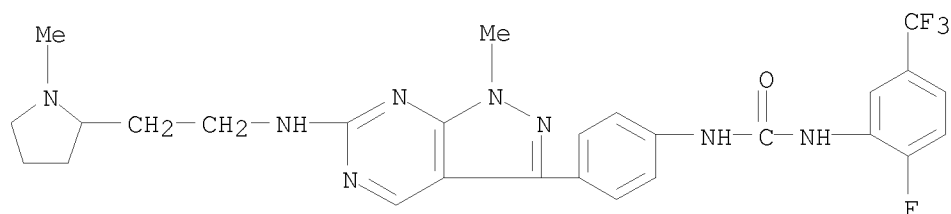
RN 508222-28-4 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[2-(1-methyl-2-pyrrolidinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-27-3

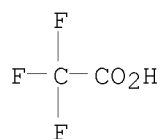
CMF C27 H28 F4 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



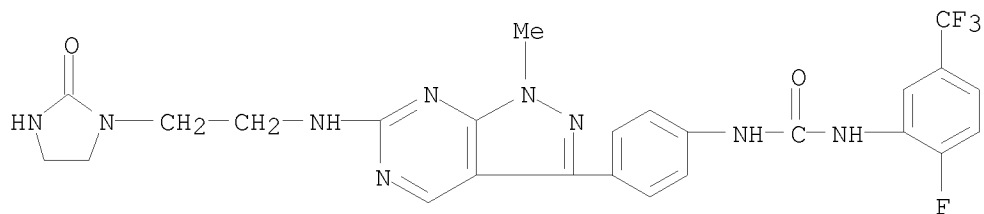
RN 508222-30-8 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[2-(2-oxo-1-imidazolidinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-29-5

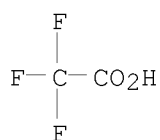
CMF C25 H23 F4 N9 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



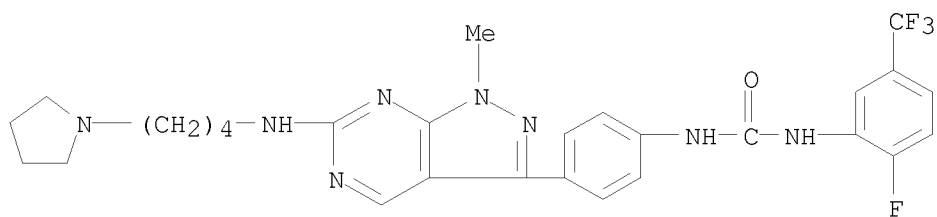
RN 508222-32-0 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[4-(1-pyrrolidinyl)butyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-31-9

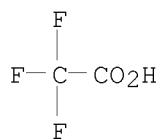
CMF C28 H30 F4 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 508222-34-2 CAPLUS

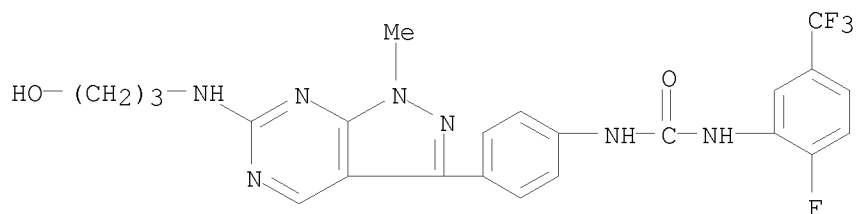
CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[6-[(3-

hydroxypropyl)amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-,
2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-33-1

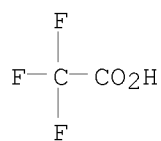
CMF C23 H21 F4 N7 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



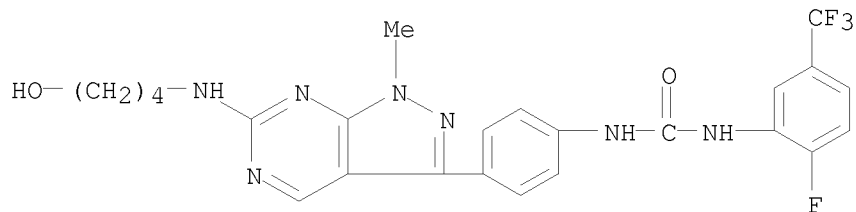
RN 508222-36-4 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[6-[(4-hydroxybutyl)amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-35-3

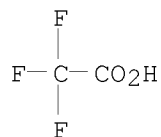
CMF C24 H23 F4 N7 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



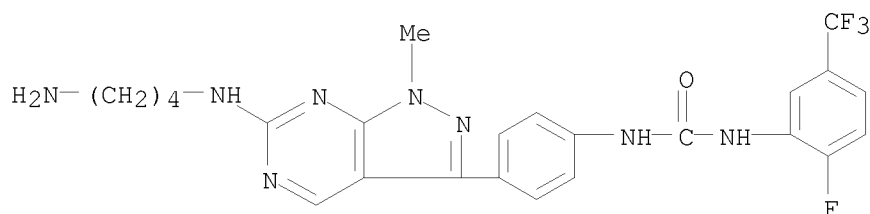
RN 508222-40-0 CAPLUS

CN Urea, N-[4-[6-[(4-aminobutyl)amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-39-7

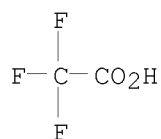
CMF C24 H24 F4 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



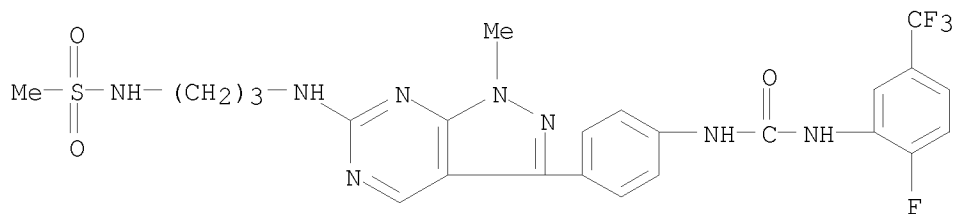
RN 508222-42-2 CAPLUS

CN Methanesulfonamide, N-[3-[3-[4-[[[2-fluoro-5-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]amino]propyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-41-1

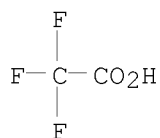
CMF C24 H24 F4 N8 O3 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



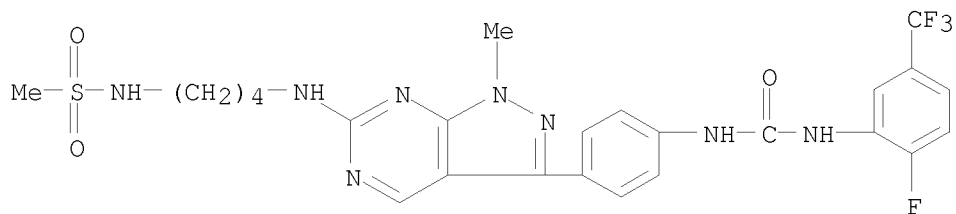
RN 508222-44-4 CAPLUS

CN Methanesulfonamide, N-[4-[[3-[4-[[[2-fluoro-5-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]amino]butyl]-, 2,2,2-trifluoroacetate (1:1)
(CA INDEX NAME)

CM 1

CRN 508222-43-3

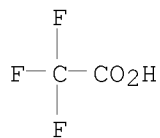
CMF C25 H26 F4 N8 O3 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



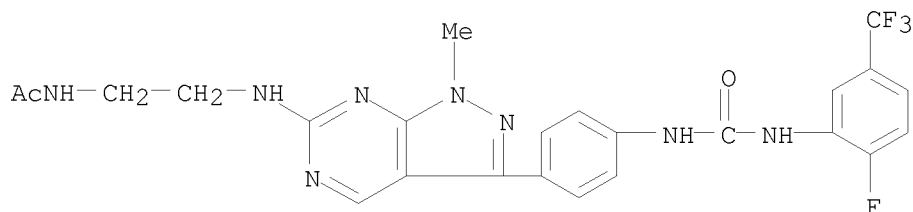
RN 508222-46-6 CAPLUS

CN Acetamide, N-[2-[[3-[4-[[[2-fluoro-5-(trifluoromethyl)phenyl]amino]carbon
yl]amino]phenyl]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-6-yl]amino]ethyl]-,
2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-45-5

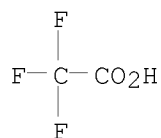
CMF C24 H22 F4 N8 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



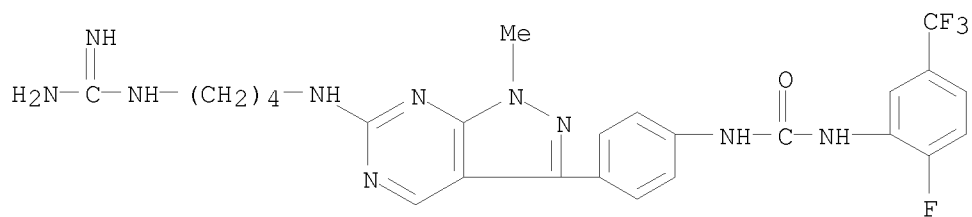
RN 508222-48-8 CAPLUS

CN Urea, N-[4-[6-[[4-[(aminoiminomethyl)amino]butyl]amino]-1-methyl-1H-
pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-
(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508222-47-7

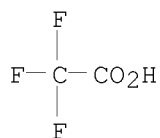
CMF C25 H26 F4 N10 O



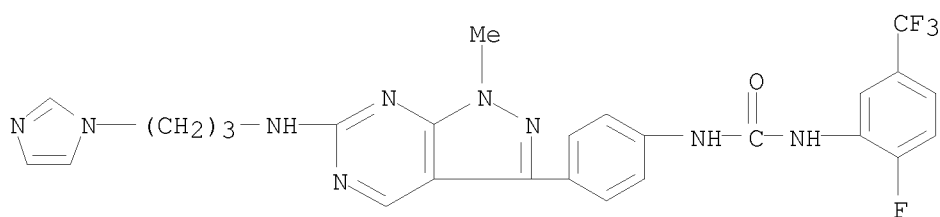
CM 2

CRN 76-05-1

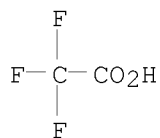
CMF C2 H F3 O2



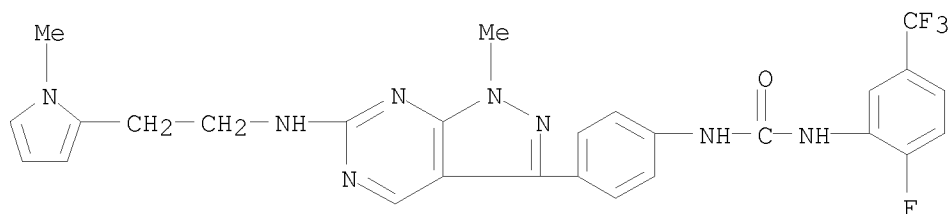
RN 508222-50-2 CAPLUS
 CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[6-[[3-(1H-imidazol-1-yl)propyl]amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)
 CM 1
 CRN 508222-49-9
 CMF C26 H23 F4 N9 O



CM 2
 CRN 76-05-1
 CMF C2 H F3 O2

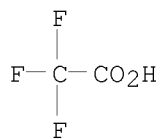


RN 508222-52-4 CAPLUS
 CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[2-(1-methyl-1H-pyrrol-2-yl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)
 CM 1
 CRN 508222-51-3
 CMF C27 H24 F4 N8 O



CM 2

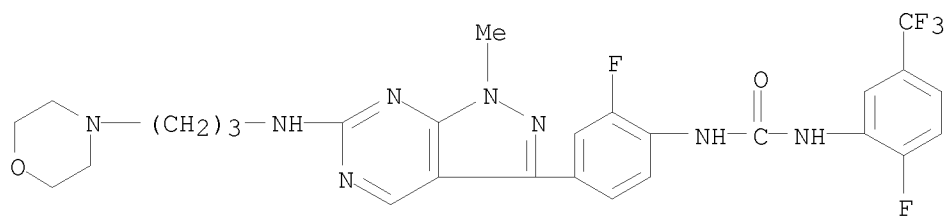
CRN 76-05-1
CMF C2 H F3 O2



RN 508222-99-9 CAPLUS
CN Urea, N-[2-fluoro-4-[1-methyl-6-[[3-(4-morpholinyl)propyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

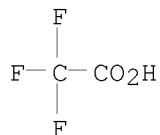
CM 1

CRN 508222-98-8
CMF C27 H27 F5 N8 O2



CM 2

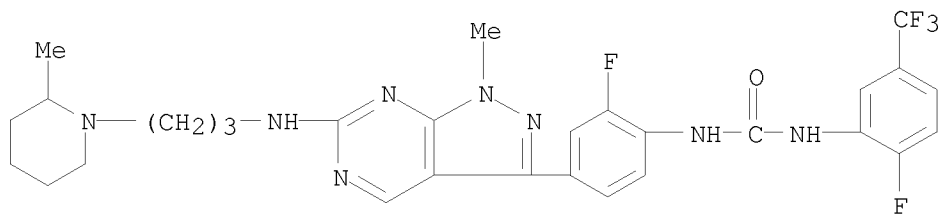
CRN 76-05-1
CMF C2 H F3 O2



RN 508223-01-6 CAPLUS
CN Urea, N-[2-fluoro-4-[1-methyl-6-[[3-(2-methyl-1-piperidiny)propyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

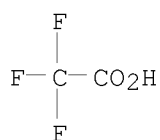
CRN 508223-00-5
CMF C29 H31 F5 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



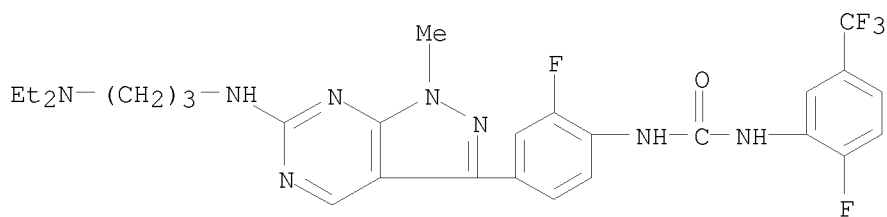
RN 508223-03-8 CAPLUS

CN Urea, N-[4-[6-[[3-(diethylamino)propyl]amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-2-fluorophenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508223-02-7

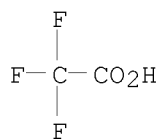
CMF C27 H29 F5 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 508223-05-0 CAPLUS

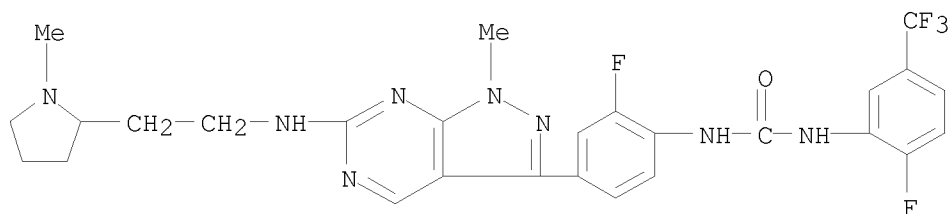
CN Urea, N-[2-fluoro-4-[1-methyl-6-[[2-(1-methyl-2-pyrrolidinyl)ethyl]amino]-

1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508223-04-9

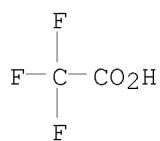
CMF C27 H27 F5 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



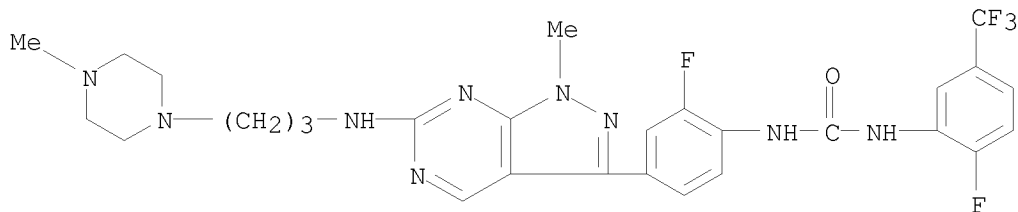
RN 508223-07-2 CAPLUS

CN Urea, N-[2-fluoro-4-[1-methyl-6-[[3-(4-methyl-1-piperazinyl)propyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508223-06-1

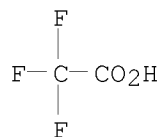
CMF C28 H30 F5 N9 O



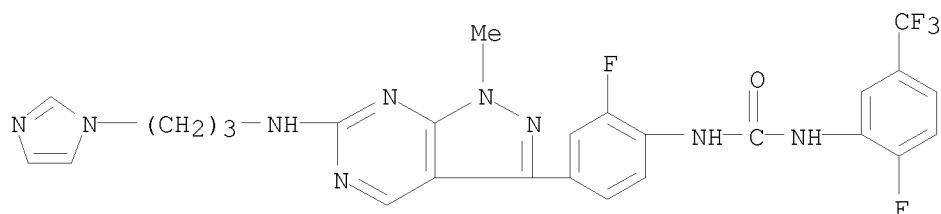
CM 2

CRN 76-05-1

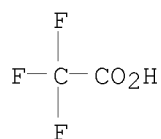
CMF C2 H F3 O2



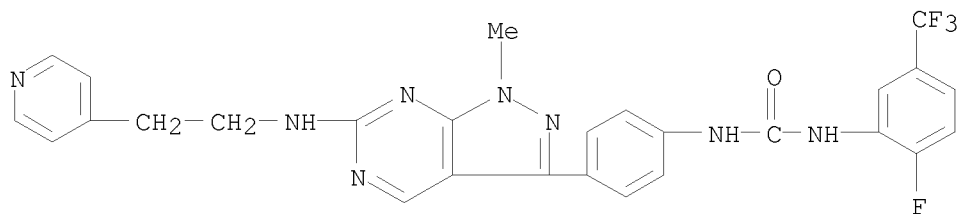
RN 508223-09-4 CAPLUS
 CN Urea, N-[2-fluoro-4-[6-[[3-(1H-imidazol-1-yl)propyl]amino]-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)
 CM 1
 CRN 508223-08-3
 CMF C26 H22 F5 N9 O



CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



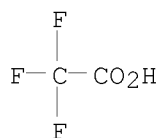
RN 508223-24-3 CAPLUS
 CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[2-(4-pyridinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)
 CM 1
 CRN 508223-23-2
 CMF C27 H22 F4 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



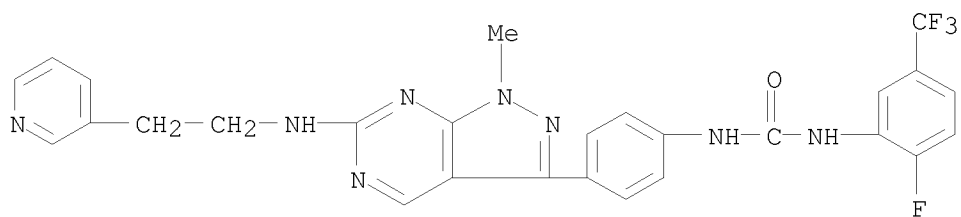
RN 508223-26-5 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[2-(3-pyridinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 508223-25-4

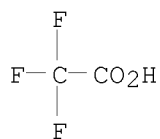
CMF C27 H22 F4 N8 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 508223-28-7 CAPLUS

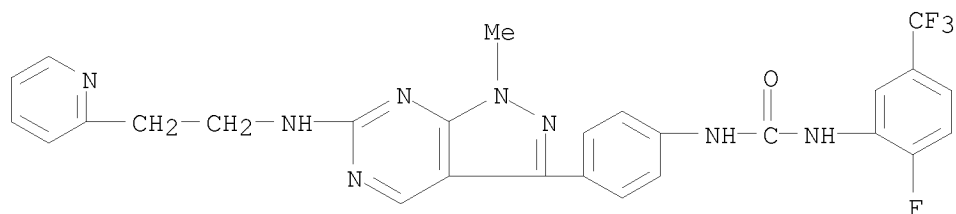
CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-[[2-(2-

pyridinyl)ethyl]amino]-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-,
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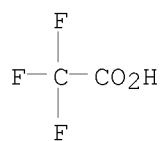
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CM 2

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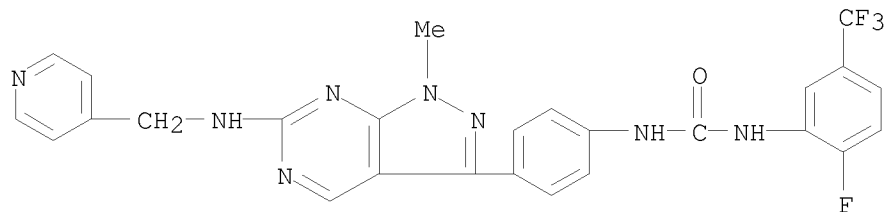
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CM 1

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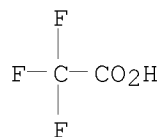
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CM 2

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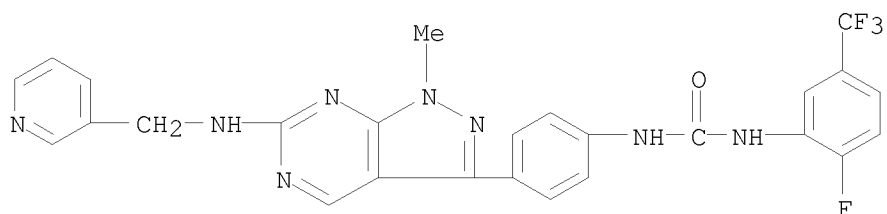
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CRN 508223-31-2

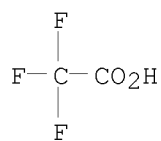
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CM 2

CRN 76-05-1

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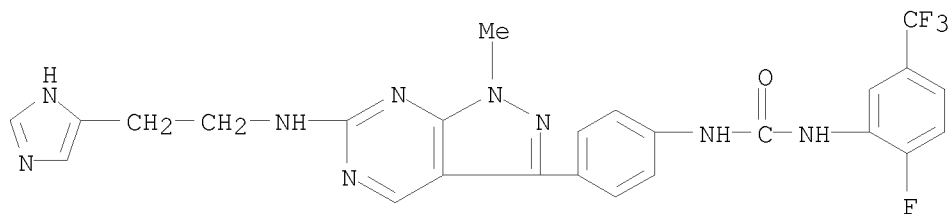
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CM 1

CRN 508223-33-4

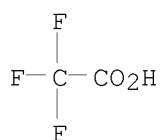
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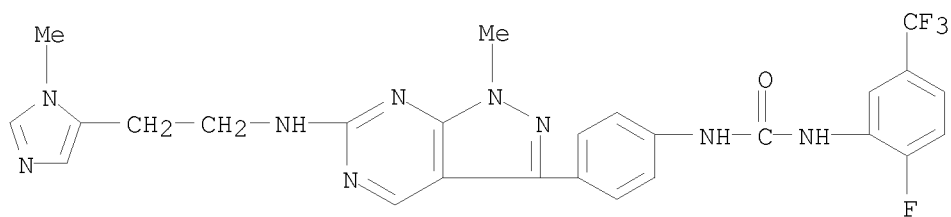
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CM 1

CRN 508223-35-6

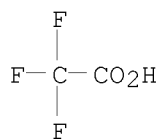
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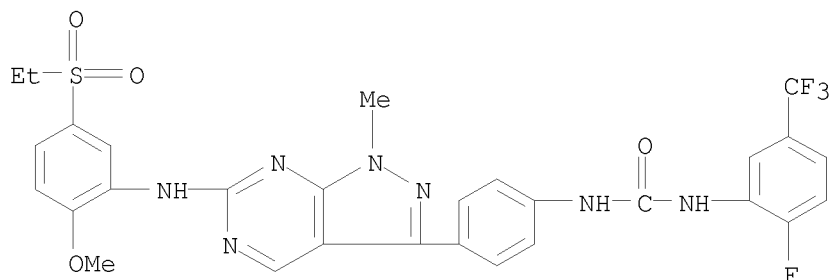
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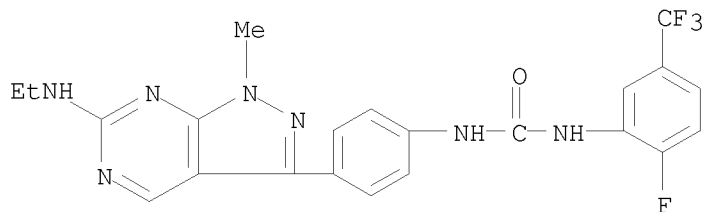
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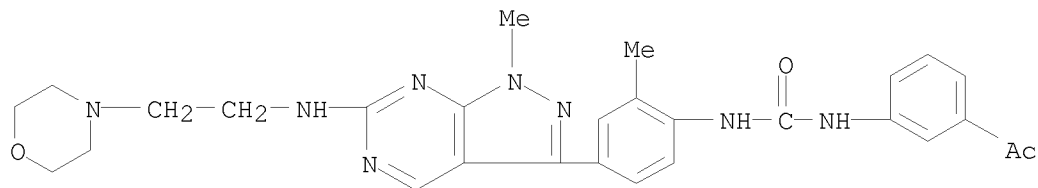
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RN 508223-52-7 CAPLUS

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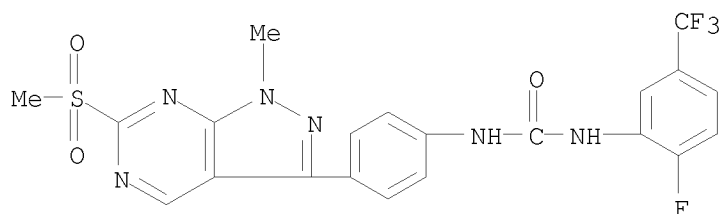
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

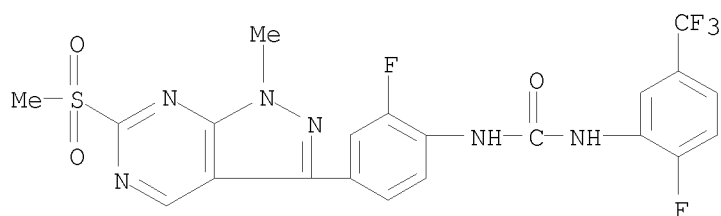
(preparation of pyrazolo[3,4-d]pyrimidine derivs. for treating diseases associated with inappropriate angiogenesis)

RN 508222-10-4 CAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[1-methyl-6-(methylsulfonyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]- (CA INDEX NAME)



RN 508222-97-7 CAPLUS
 CN Urea, N-[2-fluoro-4-[1-methyl-6-(methylsulfonyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



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L4 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:319714 CAPLUS
 DOCUMENT NUMBER: 138:338157
 TITLE: Preparation of 1,4-disubstituted benzo-fused ureas as cytokine inhibitors
 INVENTOR(S): Cirillo, Pier F.; Hammach, Abdelhakim; Regan, John R.
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 100 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003032989	A1	20030424	WO 2002-US32809	20021011
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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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US 20030162968	A1	20030828	US 2002-269173	20021011
US 6825184	B2	20041130		

EP 1438048 A1 20040721 EP 2002-801703 20021011
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IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
JP 2005506350 T 20050303 JP 2003-535792 20021011
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OTHER SOURCE(S): MARPAT 138:338157
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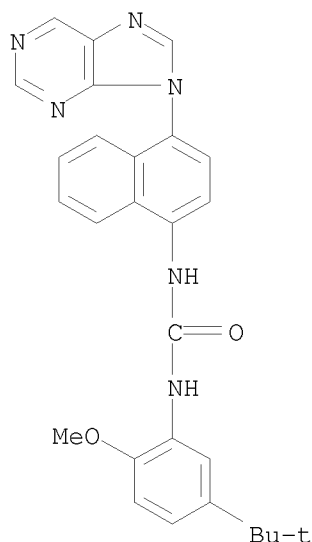
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; ring A = fused (un)saturated ring containing 3-5 carbon atoms (wherein ring A or the Ph ring to which it is fused is optionally substituted); G = (un)substituted 5-membered heteroaryl; Q = (un)substituted naphthyl, benzocyclobutanyl, indanyl, etc.; X = O, S] which are active as anti-inflammatory agents, were prepared. Thus, reacting the carbamate II with the amine III (multi-step preparation given) in DMSO afforded 84% urea IV. The preferred compds. I including those from the synthetic examples were evaluated for their inhibition of TNF α production in THP cells, and showed IC₅₀ < 10 μ M.

IT 515843-77-3P 515843-78-4P 515843-79-5P
515843-80-8P 515843-81-9P 515843-82-0P
515843-83-1P 515843-84-2P 515843-85-3P
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515844-04-9P 515844-05-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,4-disubstituted benzo-fused ureas as cytokine inhibitors)

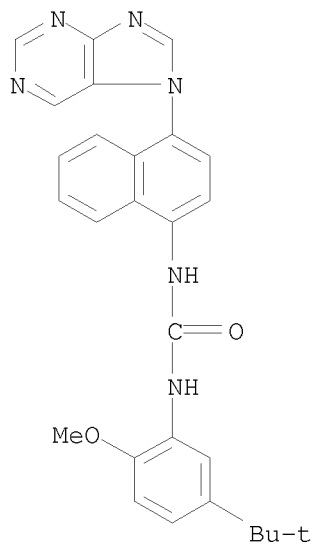
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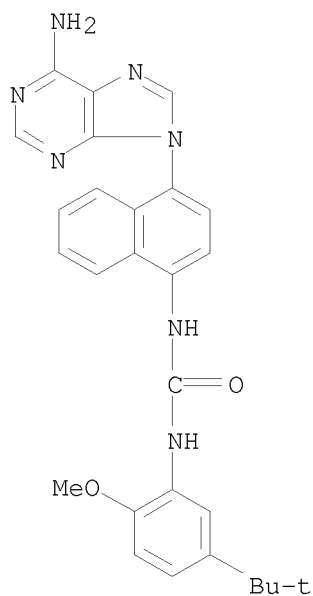
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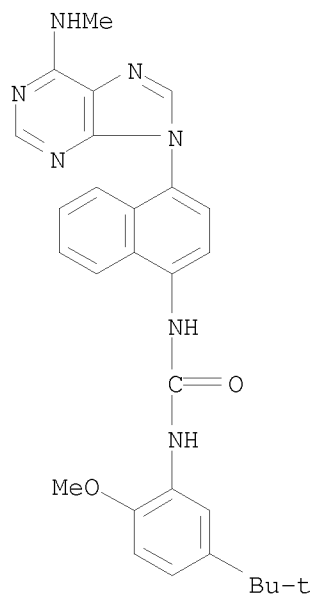
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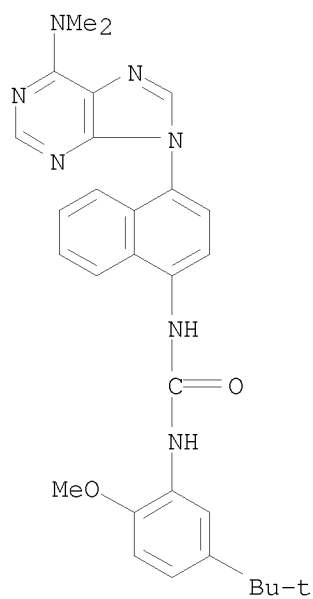
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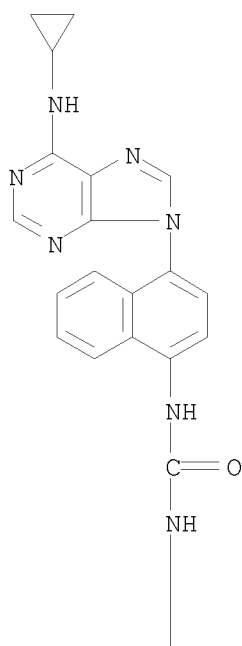
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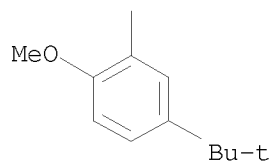
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CN Urea, N-[4-[6-(cyclopropylamino)-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

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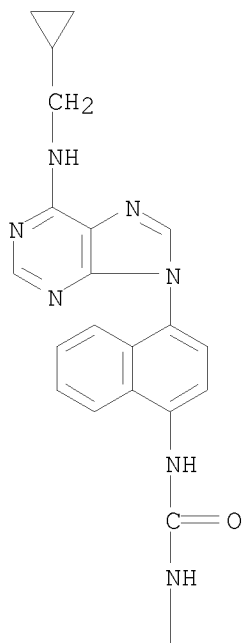


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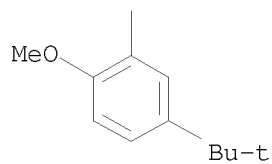


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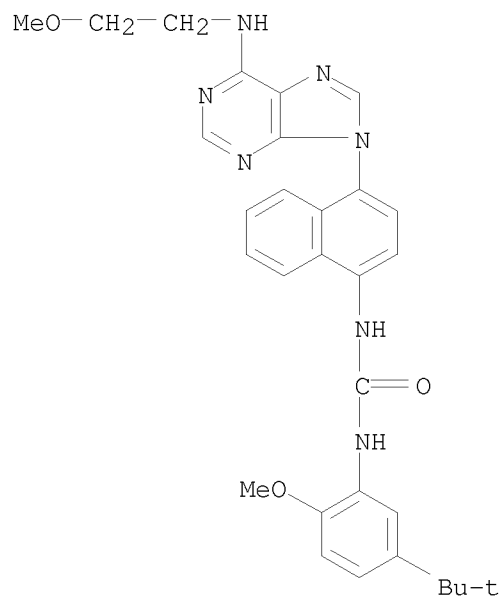
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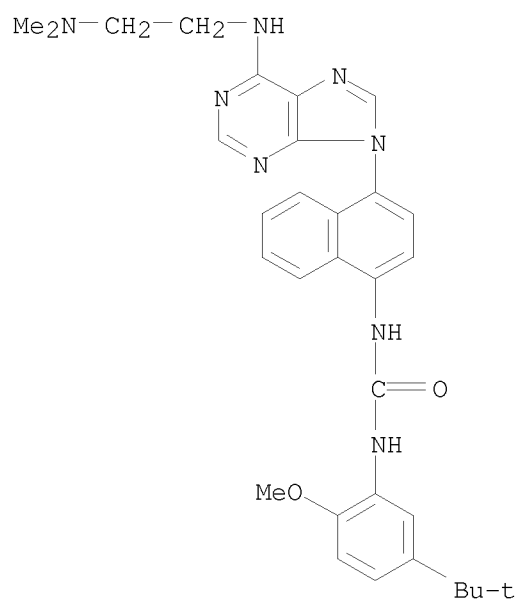
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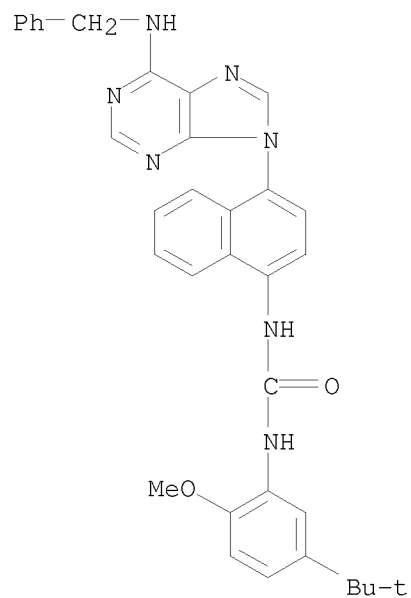
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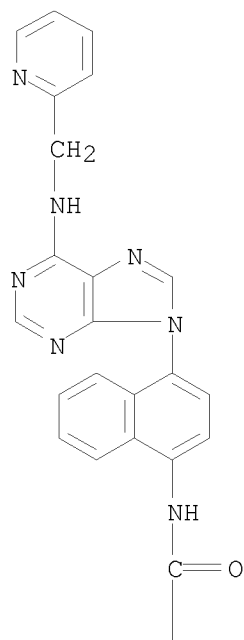


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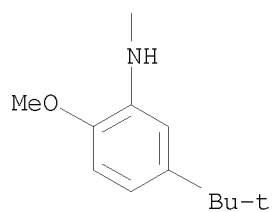


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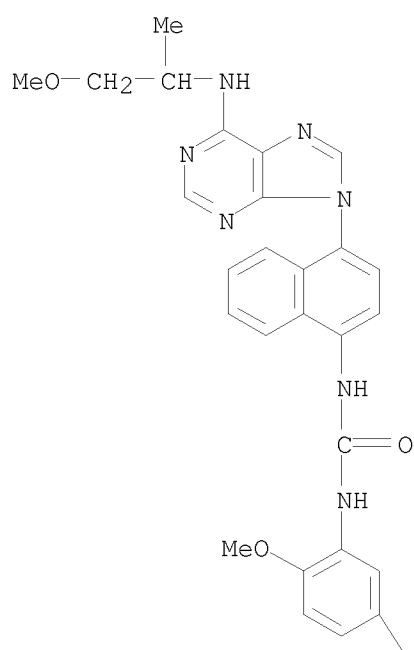


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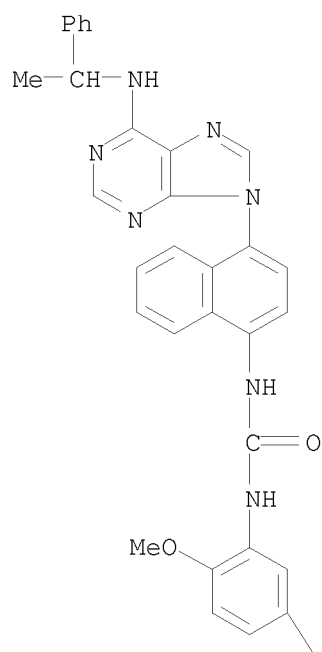


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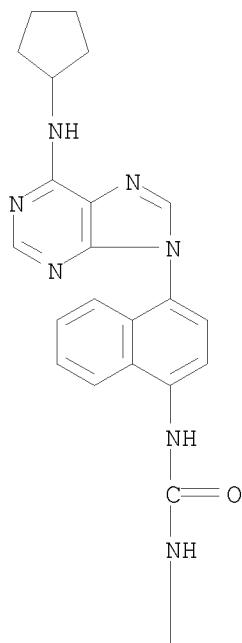


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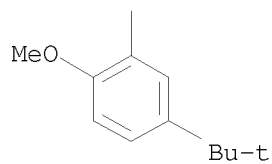


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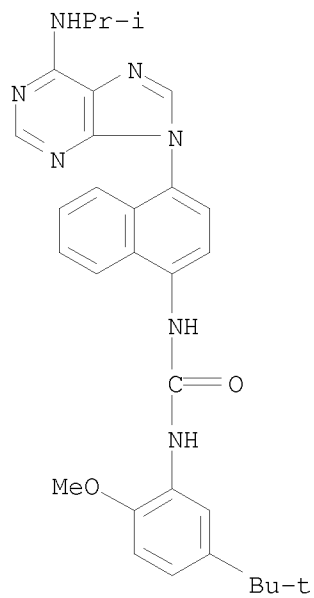
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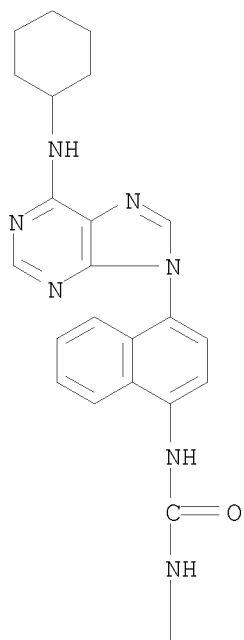


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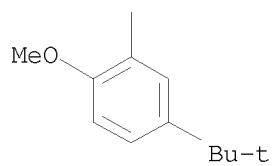


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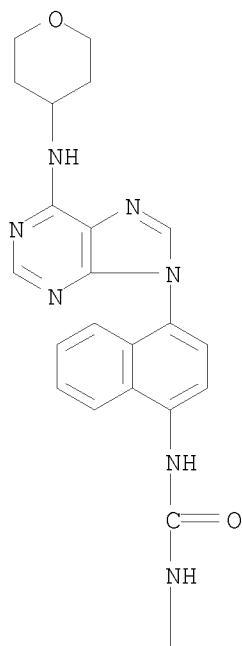


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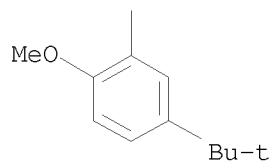


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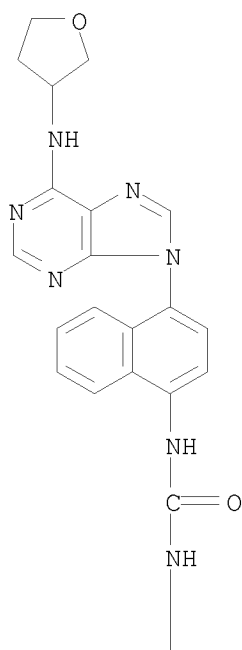


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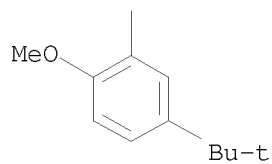


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CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[(tetrahydro-3-furanyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

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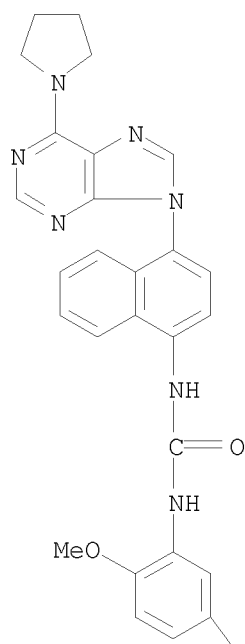


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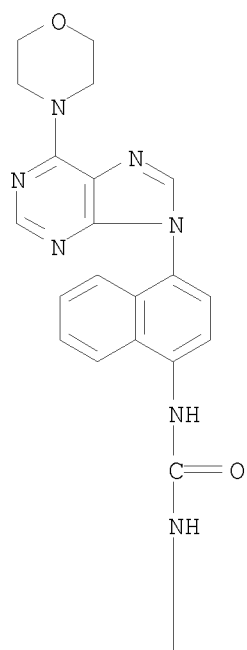


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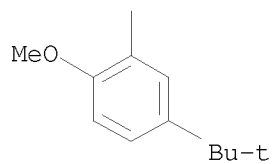
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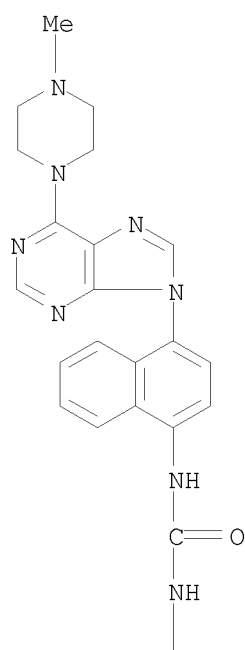


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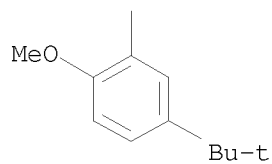


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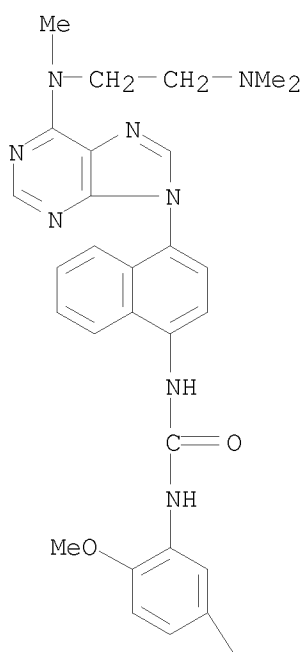


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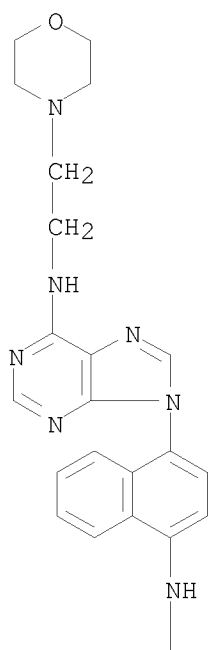


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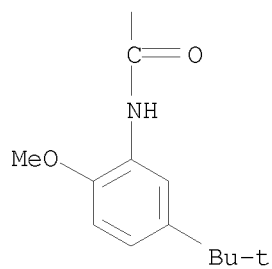


RN 515843-99-9 CAPLUS
CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[[2-(4-morpholinyl)ethyl]amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

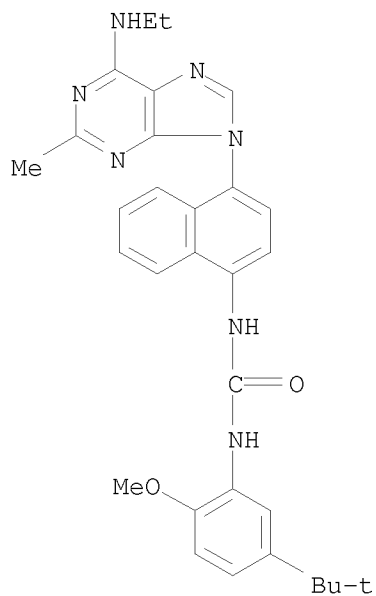
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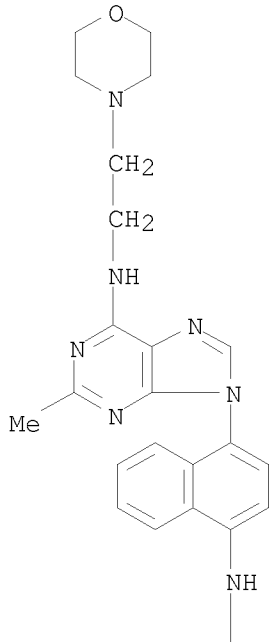


RN 515844-00-5 CAPLUS
CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(ethylamino)-2-methyl-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

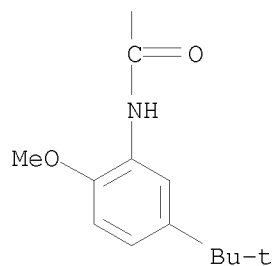


RN 515844-01-6 CAPLUS
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PAGE 1-A

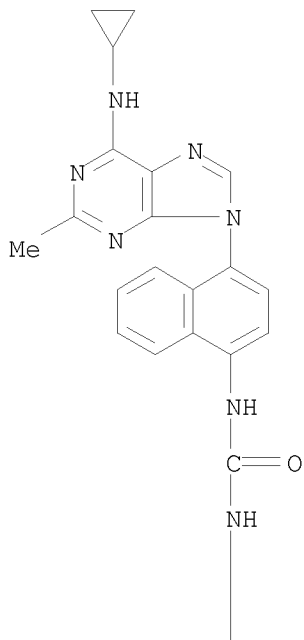


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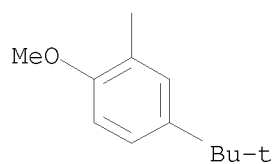


RN 515844-02-7 CAPLUS
CN Urea, N-[4-[6-(cyclopropylamino)-2-methyl-9H-purin-9-yl]-1-naphthalenyl]-
N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

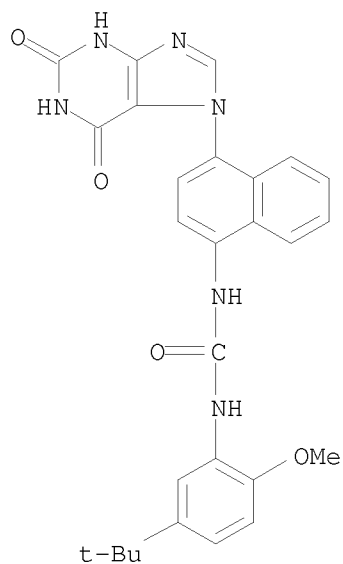
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PAGE 2-A

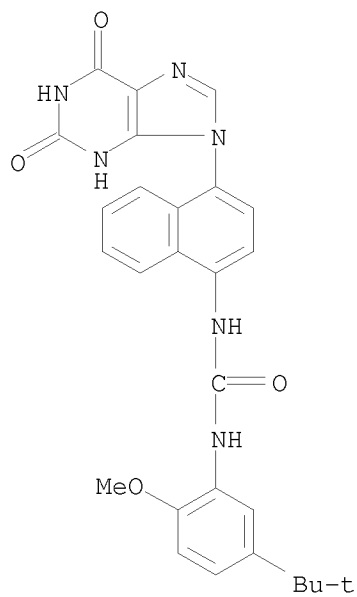


RN 515844-03-8 CAPLUS
CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-(1,2,3,6-tetrahydro-
2,6-dioxo-7H-purin-7-yl)-1-naphthalenyl]- (CA INDEX NAME)



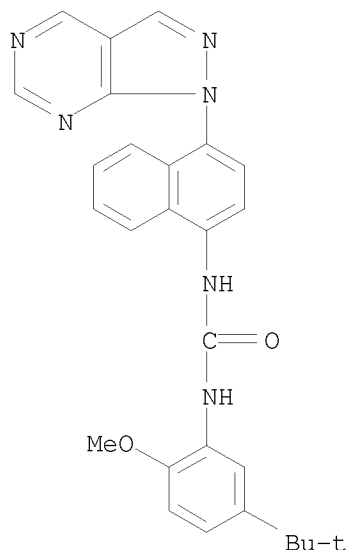
RN 515844-04-9 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-(1,2,3,6-tetrahydro-2,6-dioxo-9H-purin-9-yl)-1-naphthalenyl]- (CA INDEX NAME)



RN 515844-05-0 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-(1H-pyrazolo[3,4-d]pyrimidin-1-yl)-1-naphthalenyl]- (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:125101 CAPLUS

DOCUMENT NUMBER: 140:339109

TITLE: Design, Synthesis, and Biological Evaluation of New 8-Heterocyclic Xanthine Derivatives as Highly Potent and Selective Human A2B Adenosine Receptor Antagonists

AUTHOR(S): Baraldi, Pier Giovanni; Tabrizi, Mojgan Aghazadeh; Preti, Delia; Bovero, Andrea; Romagnoli, Romeo; Fruttarolo, Francesca; Zaid, Naser Abdel; Moorman, Allan R.; Varani, Katia; Gessi, Stefania; Merighi, Stefania; Borea, Pier Andrea

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Dipartimento di Medicina Clinica e Sperimentale-Sezione di Farmacologia, Universita di Ferrara, Ferrara, 44100, Italy

SOURCE: Journal of Medicinal Chemistry (2004), 47(6), 1434-1447

CODEN: JMCMAR; ISSN: 0022-2623

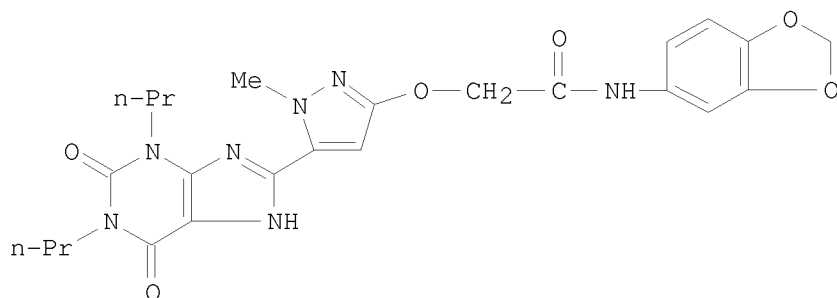
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:339109

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I

AB The synthesis of 8-heterocycle-substituted xanthines as potent and selective A2B adenosine receptor antagonists was reported. The structure-activity relationships (SAR) of the xanthines synthesized in binding to recombinant human A2B adenosine receptors (ARs) in HEK-293 cells (HEK-A2B) and at other AR subtypes were explored. The synthesized compds. showed A2B adenosine receptor affinity in the nanomolar range and good levels of selectivity evaluated in radioligand binding assays at human (h) A1, A2A, A2B, and A3 ARs. Several heterocycles, such as pyrazole, isoxazole, pyridine, and pyridazine, were introduced at the 8-position of the xanthine nucleus and different spacers (substituted acetamide, oxyacetamide, and urea moieties) were investigated. Various groups at the 3- and 4-positions of phenylacetamide moiety were studied. This study allowed us to identify 2-(3,4-dimethoxyphenyl)-N-[5-(2,6-dioxo-1,3-dipropyl-2,3,6,7-tetrahydro-1H-purin-8-yl)-1-methyl-1H-pyrazol-3-yl]acetamide (MRE2028F20) [Ki(hA2B) = 38 nM, Ki(hA1,hA2A,hA3) >1000 nM], N-1,3-benzodioxol-5-yl-2-[[1-methyl-5-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)-1H-pyrazol-3-yl]oxy]acetamide (I, MRE2029F20) [Ki(hA2B) = 5.5 nM, Ki(hA1,hA2A,hA3) > 1000 nM], and N-(3,4-dimethoxyphenyl)-2-[5-(2,6-dioxo-1,3-dipropyl-2,3,6,7-tetrahydro-1H-purin-8-yl)-1-methyl-1H-pyrazol-3-yloxy]acetamide (MRE2030F20) [Ki(hA2B) = 12 nM, Ki(hA1,hA2A, hA3) > 1000 nM], which showed high affinity at the A2B receptor subtype and very good selectivity vs the other ARs. Substitution of the acetamide with an urea moiety afforded bioisosteric xanthines with good affinity and selectivity comparable to the acetamide derivs. Substitution at the para-position of a 4-benzyloxy group of the phenylacetamido chain enhanced affinity at the A2B receptor but did not favor selectivity. The derivs. with higher affinity at human A2B AR proved to be antagonists, in the cAMP assay, capable of inhibiting the stimulatory effect of NECA (100 nM) with IC50 values in the nanomolar range, a trend similar to that observed in the binding assay for I (IC50 = 38 nM) for MRE2029F20 (IC50 = 46 nM). In conclusion, the 8-pyrazolo-1,3-dipropyl-1H-purine-2,6-dione derivs. described herein represent a new family of selective antagonists for the adenosine A2B receptor.

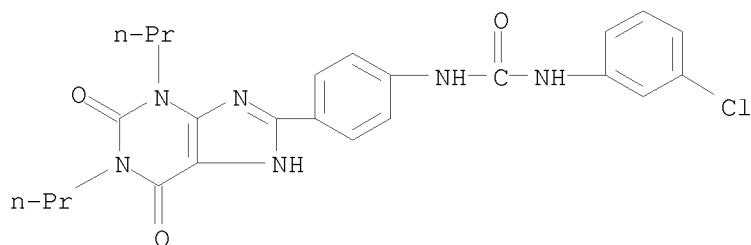
IT 679436-50-1P 679436-51-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

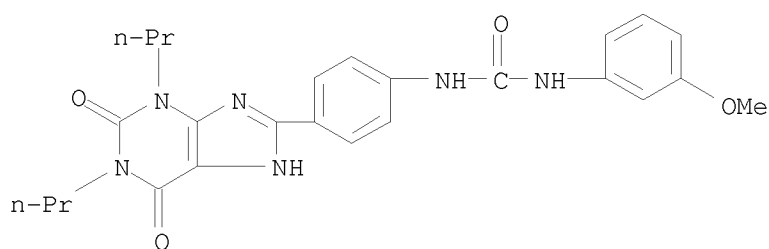
(design, synthesis, and evaluation of heterocyclic xanthine derivs. as highly potent and selective human A2B adenosine receptor antagonists)

RN 679436-50-1 CAPLUS

CN Urea, N-(3-chlorophenyl)-N'-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenyl]- (CA INDEX NAME)



RN 679436-51-2 CAPLUS
 CN Urea, N-(3-methoxyphenyl)-N'-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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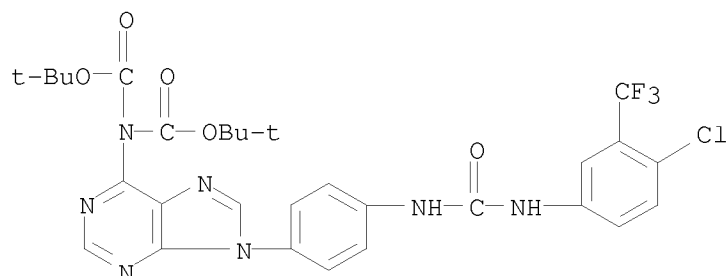
L4 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:962206 CAPLUS
 DOCUMENT NUMBER: 143:266944
 TITLE: Preparation of heteroarylphenylurea derivatives as Raf inhibitors
 INVENTOR(S): Oikawa, Nobuhiro; Mizuguchi, Eisaku; Morikami, Kenji; Shimma, Nobuo; Ishii, Nobuya; Tsukaguchi, Toshiyuki; Ozawa, Sawako
 PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan
 SOURCE: PCT Int. Appl., 296 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005080330	A1	20050901	WO 2005-JP2923	20050223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,				

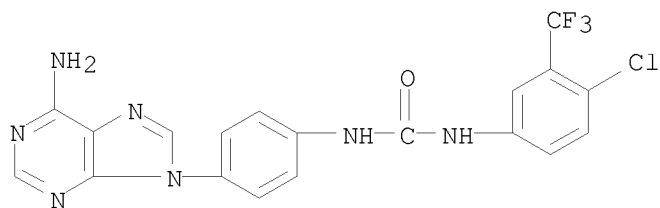
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US 20080119466 A1 20080522 US 2006-590026 20060818
PRIORITY APPLN. INFO.: JP 2004-47037 A 20040223
JP 2004-248856 A 20040827
WO 2005-JP2923 W 20050223
OTHER SOURCE(S): MARPAT 143:266944
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1, R2, R5 = H, halo, etc.; R3, R4 = H, halo, etc.; R6,
R7 = H, halo; Z1, Z2 = H, OH, etc.; Q = II; G1 = C-Y2, N; ring A =
benzene, etc.; Y1, Y2 = H, halo, etc.] were prepared For example, treatment
of 1-[4-(6-aminopurin-9-yl)phenyl]-3-[4-chloro-3-
(trifluoromethyl)phenyl]urea hydrochloride, e.g., prepared from adenine in 5
steps, with propylisocyanate afforded compound III. In Raf-1 enzyme
inhibition assays, the IC50 value of compound III was 0.013 μ M.
Cpmpounds I are claimed useful for the treatment of cancer, diabetes, etc.
IT 863673-35-2P 863673-36-3P 863673-42-1P
863673-54-5P 863673-58-9P 863673-68-1P
863674-28-6P 863674-35-5P 863674-36-6P
863674-48-0P 863674-50-4P 863674-56-0P
863674-57-1P 863674-58-2P 863675-11-0P
863675-12-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of heteroarylphenylurea derivs. as Raf inhibitors for treatment
of cancer and diabetes)
RN 863673-35-2 CAPLUS
CN Imidodicarbonic acid, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino
]carbonyl]amino]phenyl]-9H-purin-6-yl]-, C,C'-bis(1,1-dimethylethyl) ester
(CA INDEX NAME)

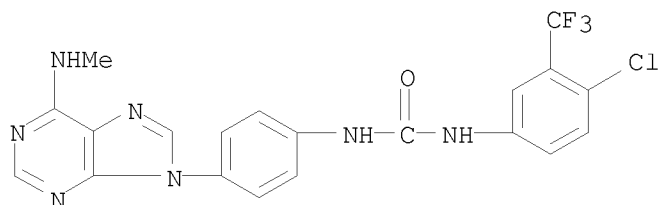


RN 863673-36-3 CAPLUS
CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-
(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



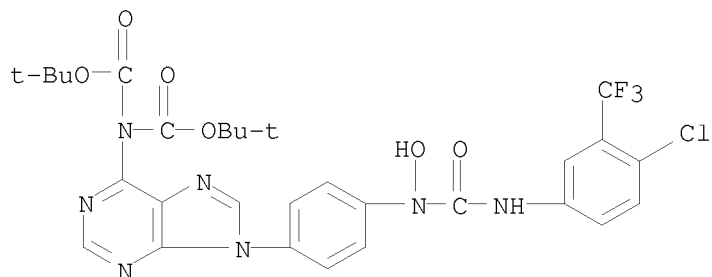
● HCl

RN 863673-42-1 CAPLUS
 CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methyamino)-9H-purin-9-yl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

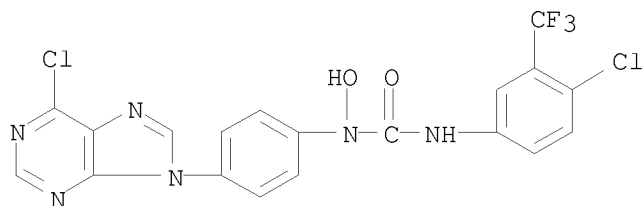


● HCl

RN 863673-54-5 CAPLUS
 CN Imidodicarbonic acid, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]hydroxyamino]phenyl]-9H-purin-6-yl]-, C,C'-bis(1,1-dimethylethyl) ester (CA INDEX NAME)

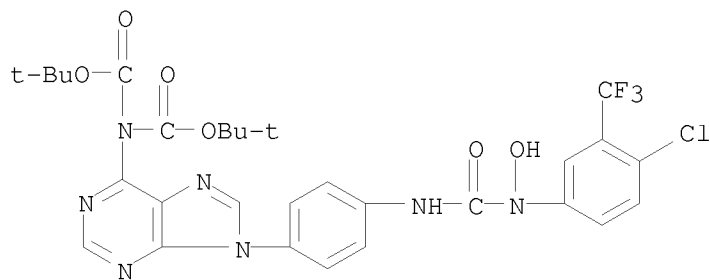


RN 863673-58-9 CAPLUS
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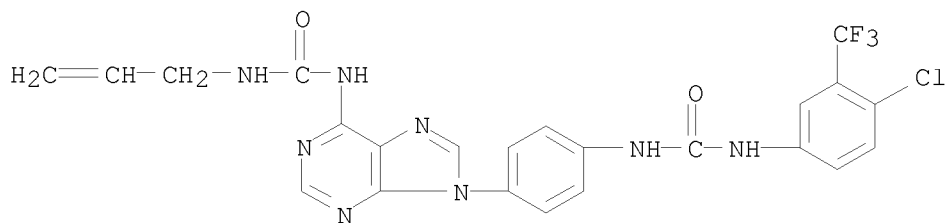
RN 863673-68-1 CAPLUS

CN Imidodicarbonic acid, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]hydroxyamino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, C,C'-bis(1,1-dimethylethyl) ester (CA INDEX NAME)



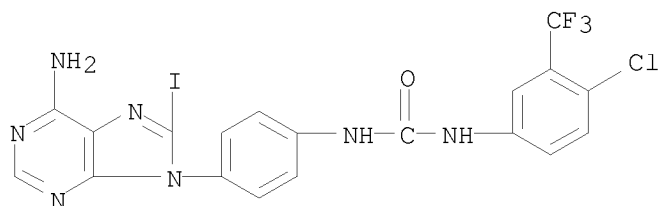
RN 863674-28-6 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-2-propen-1-yl- (CA INDEX NAME)



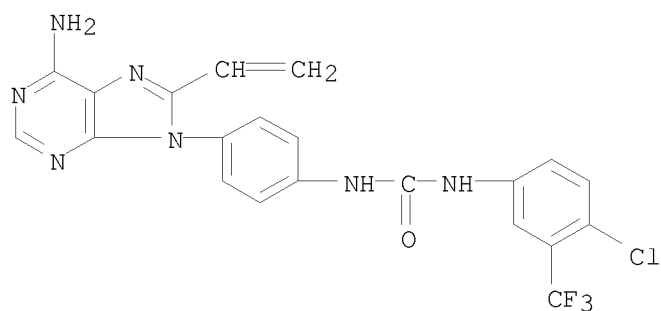
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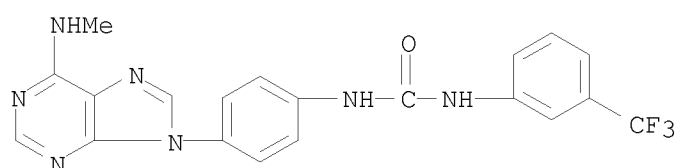
RN 863674-36-6 CAPLUS

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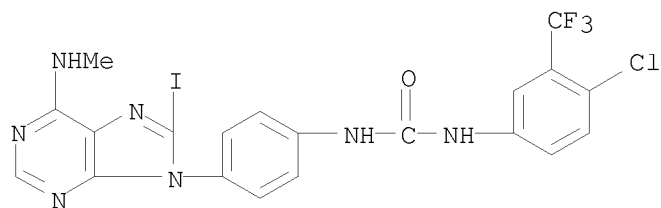
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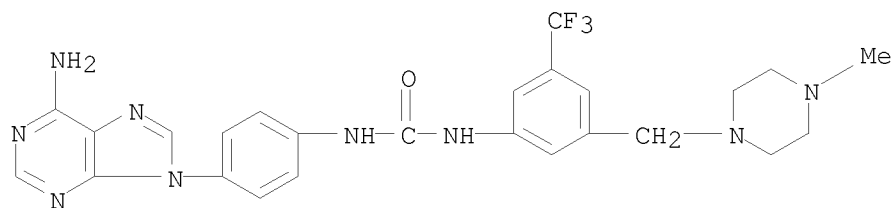
RN 863674-50-4 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-iodo-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



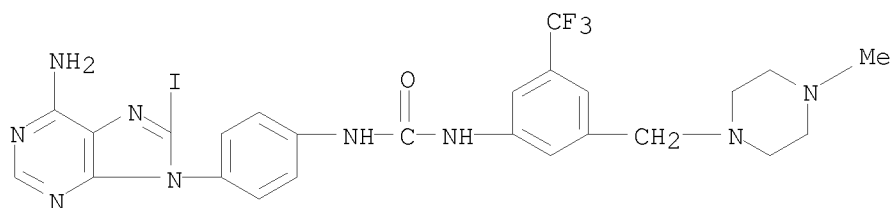
RN 863674-56-0 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



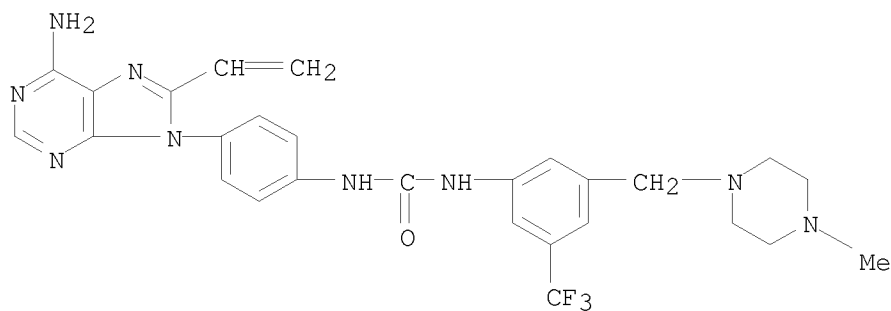
RN 863674-57-1 CAPLUS

CN Urea, N-[4-(6-amino-8-iodo-9H-purin-9-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



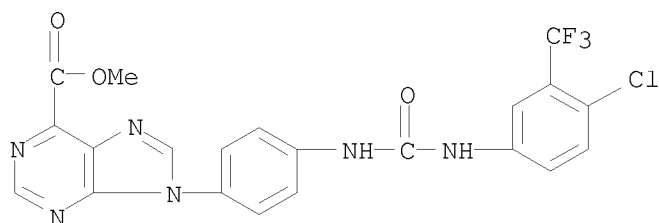
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CN Urea, N-[4-(6-amino-8-ethenyl-9H-purin-9-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



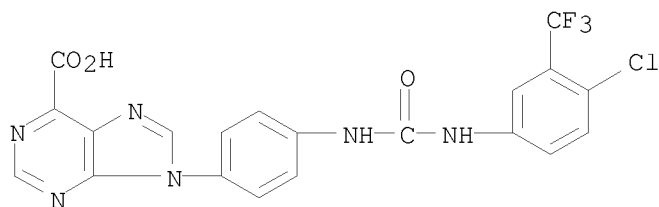
RN 863675-11-0 CAPLUS

CN 9H-Purine-6-carboxylic acid, 9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-, methyl ester (CA INDEX NAME)



RN 863675-12-1 CAPLUS

CN 9H-Purine-6-carboxylic acid, 9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]- (CA INDEX NAME)



IT 863673-10-3P 863673-11-4P 863673-37-4P
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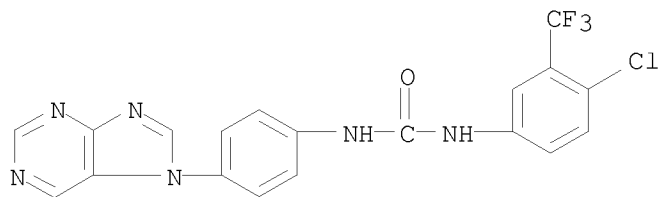
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 863675-55-2P 863675-56-3P 863675-57-4P
 863675-58-5P 863675-59-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of heteroarylphenylurea derivs. as Raf inhibitors for treatment
 of cancer and diabetes)

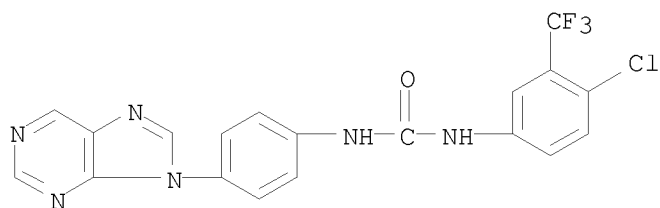
RN 863673-10-3 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-(7H-purin-7-yl)phenyl]-
 (CA INDEX NAME)



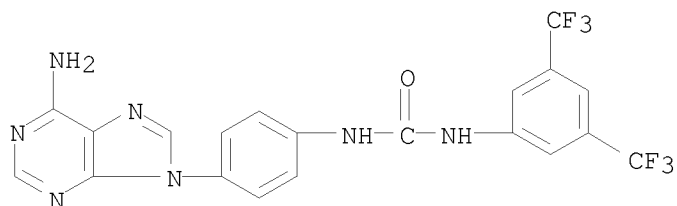
RN 863673-11-4 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-(9H-purin-9-yl)phenyl]-
(CA INDEX NAME)



RN 863673-37-4 CAPLUS

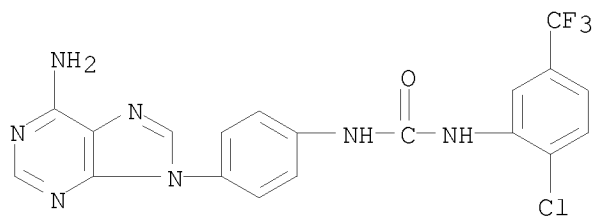
CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3,5-bis(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 863673-38-5 CAPLUS

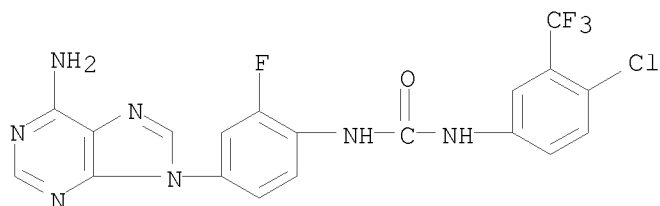
CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-chloro-5-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 863673-39-6 CAPLUS

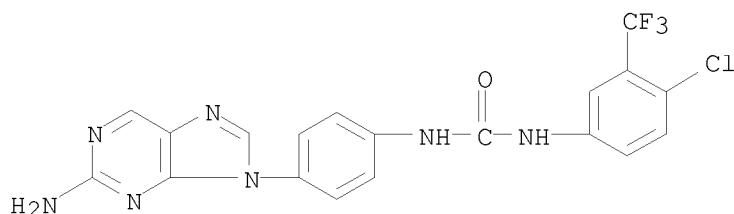
CN Urea, N-[4-(6-amino-9H-purin-9-yl)-2-fluorophenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 863673-40-9 CAPLUS

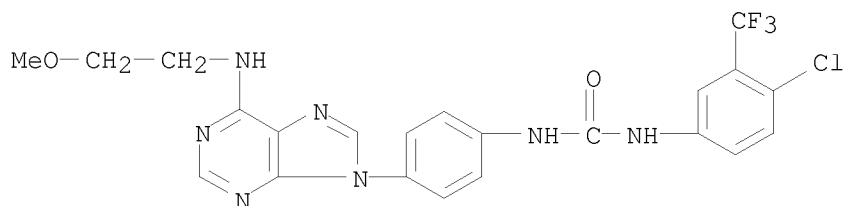
CN Urea, N-[4-(2-amino-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 863673-41-0 CAPLUS

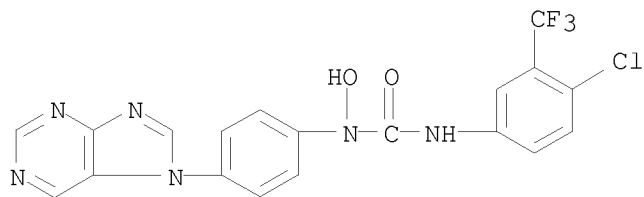
CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-[(2-methoxyethyl)amino]-9H-purin-9-yl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

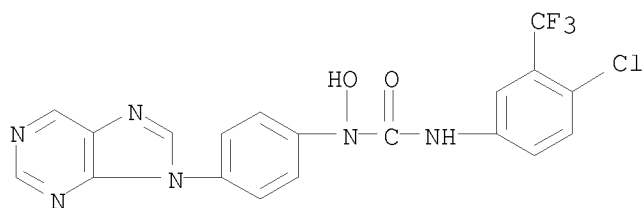
RN 863673-52-3 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-(7H-purin-7-yl)phenyl]- (CA INDEX NAME)



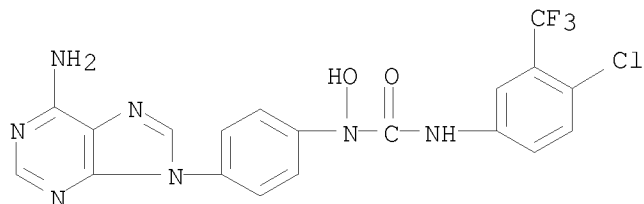
RN 863673-53-4 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-(9H-purin-9-yl)phenyl]- (CA INDEX NAME)



RN 863673-55-6 CAPLUS

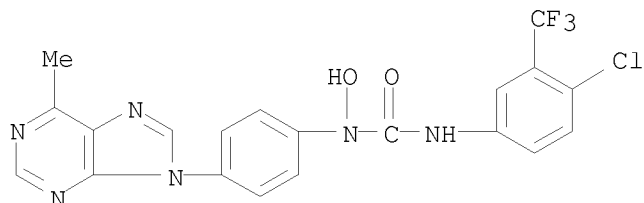
CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

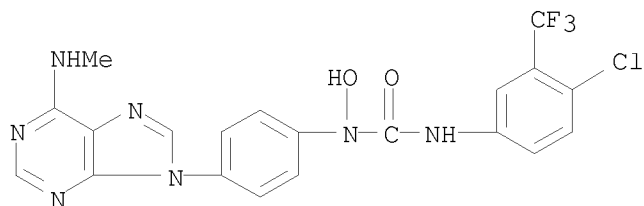
RN 863673-56-7 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-(6-methyl-9H-purin-9-yl)phenyl]- (CA INDEX NAME)



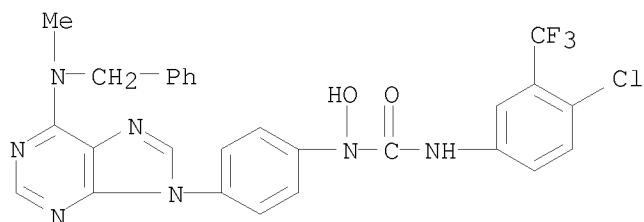
RN 863673-59-0 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



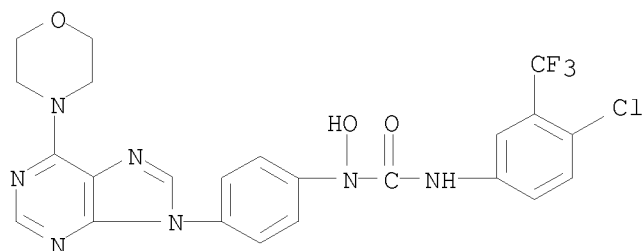
RN 863673-60-3 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-[6-[methyl(phenylmethyl)amino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



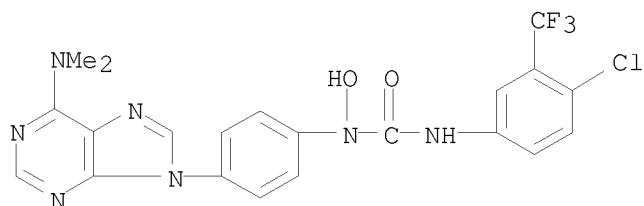
RN 863673-61-4 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-[6-(4-morpholinyl)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



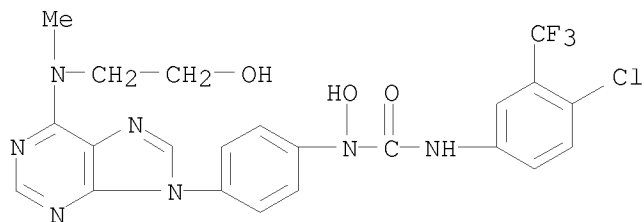
RN 863673-62-5 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-[4-[6-(dimethylamino)-9H-purin-9-yl]phenyl]-N-hydroxy- (CA INDEX NAME)



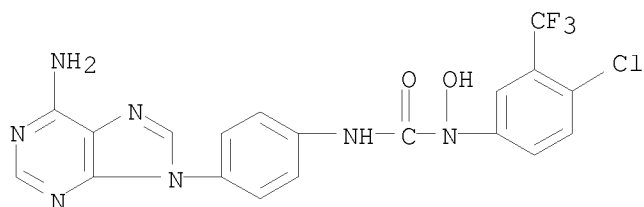
RN 863673-63-6 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-[6-[(2-hydroxyethyl)methylamino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



RN 863673-69-2 CAPLUS

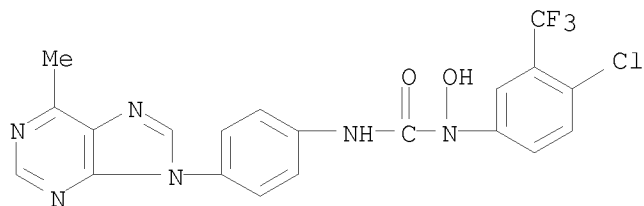
CN Urea, N'-[4-(6-amino-9H-purin-9-yl)phenyl]-N-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

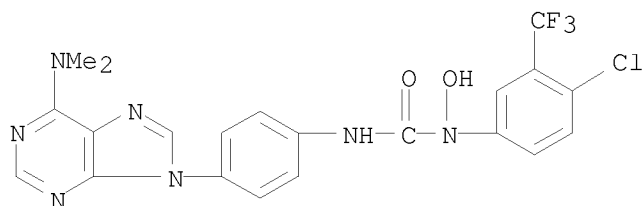
RN 863673-72-7 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N'-[4-(6-methyl-9H-purin-9-yl)phenyl]- (CA INDEX NAME)



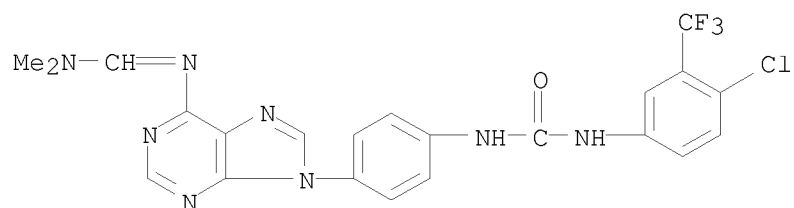
RN 863673-74-9 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(dimethylamino)-9H-purin-9-yl]phenyl]-N-hydroxy- (CA INDEX NAME)



RN 863674-01-5 CAPLUS

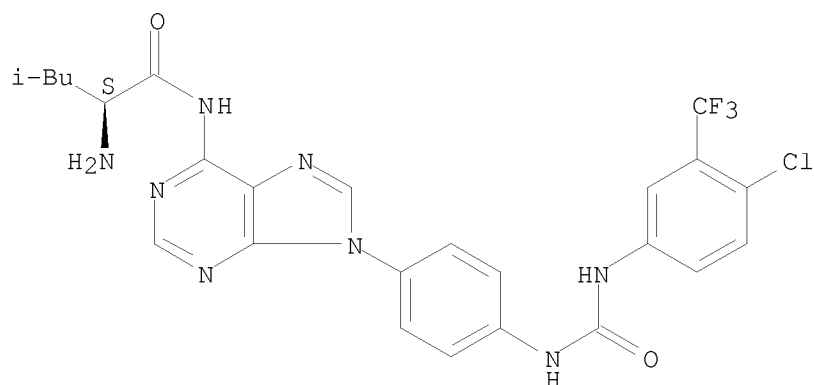
CN Methanimidamide, N'-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N,N-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

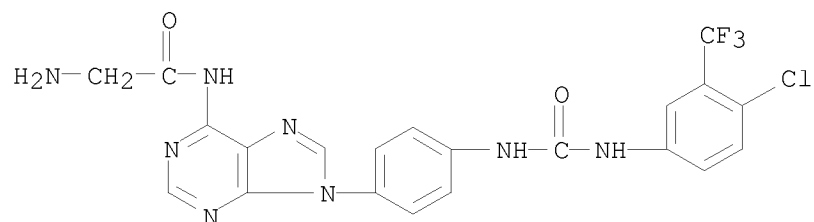
RN 863674-02-6 CAPLUS
 CN Pentanamide, 2-amino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-4-methyl-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

Absolute stereochemistry.



● HCl

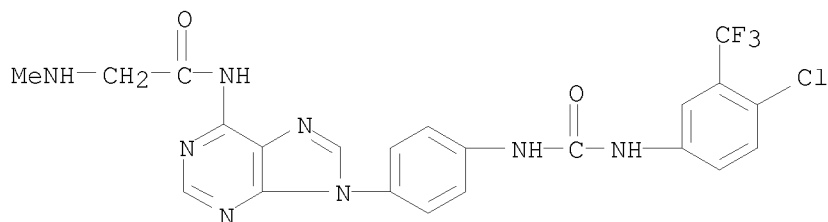
RN 863674-03-7 CAPLUS
 CN Acetamide, 2-amino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 863674-04-8 CAPLUS
 CN Acetamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]a

mino]phenyl]-9H-purin-6-yl]-2-(methylamino)-, hydrochloride (1:1) (CA INDEX NAME)

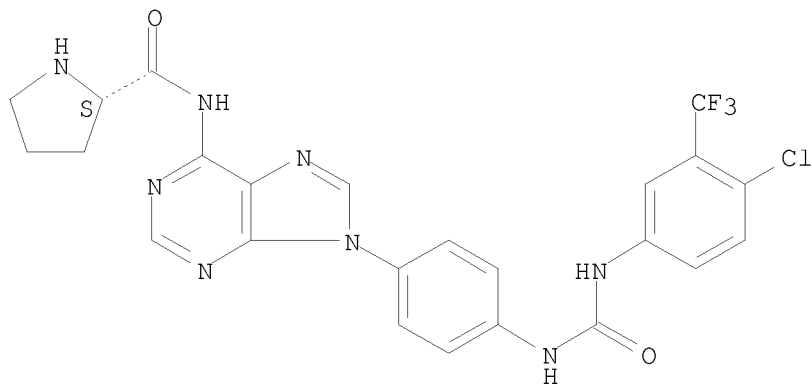


● HCl

RN 863674-05-9 CAPLUS

CN 2-Pyrrolidinecarboxamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

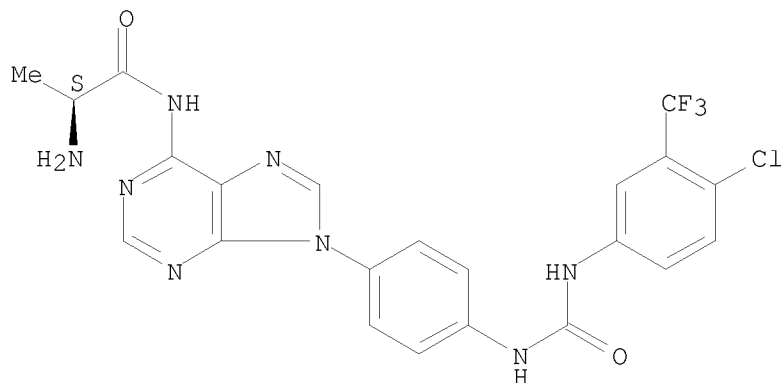


● HCl

RN 863674-06-0 CAPLUS

CN Propanamide, 2-amino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

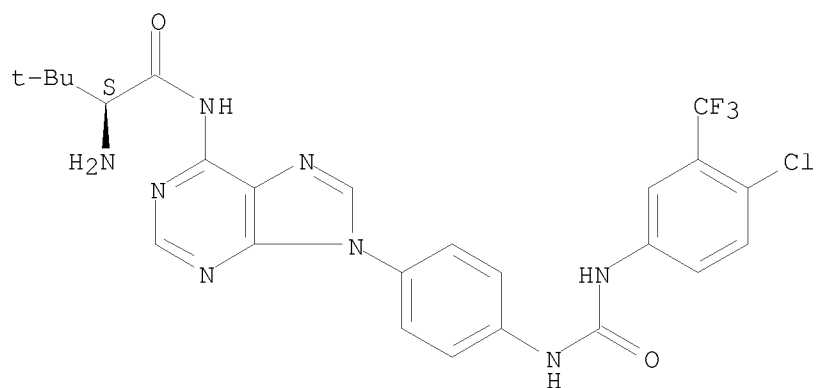
Absolute stereochemistry.



● HCl

RN 863674-07-1 CAPLUS
 CN Butanamide, 2-amino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-3,3-dimethyl-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

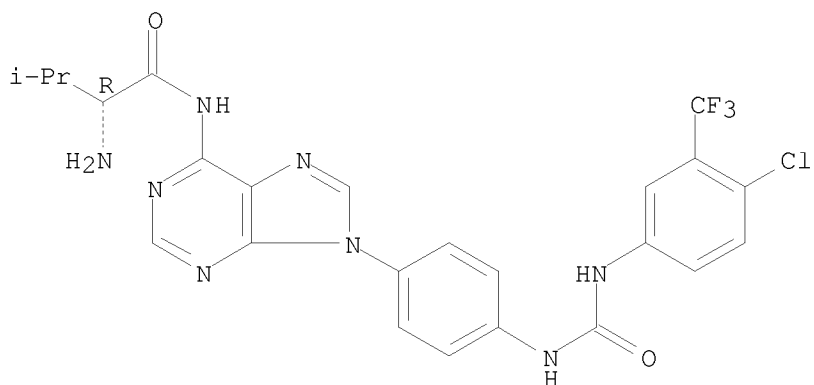
Absolute stereochemistry.



● HCl

RN 863674-08-2 CAPLUS
 CN Butanamide, 2-amino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-3-methyl-, hydrochloride (1:1), (2R)- (CA INDEX NAME)

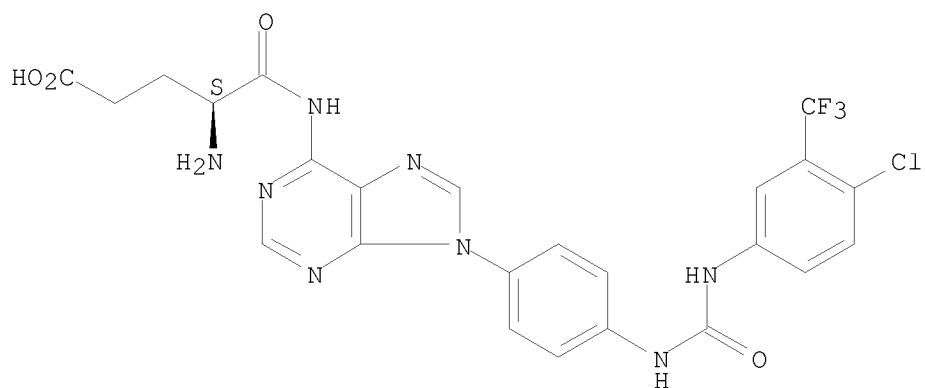
Absolute stereochemistry.



● HCl

RN 863674-09-3 CAPLUS
 CN Pentanoic acid, 4-amino-5-[[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]amino]-5-oxo-, hydrochloride (1:1), (4S)- (CA INDEX NAME)

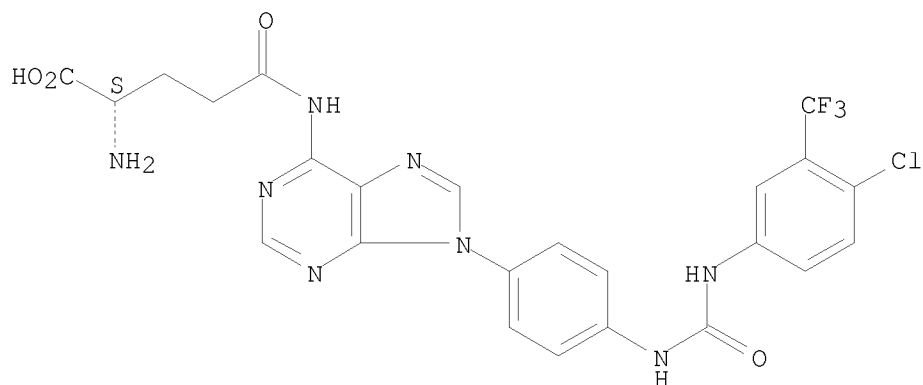
Absolute stereochemistry.



● HCl

RN 863674-10-6 CAPLUS
 CN L-Glutamine, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

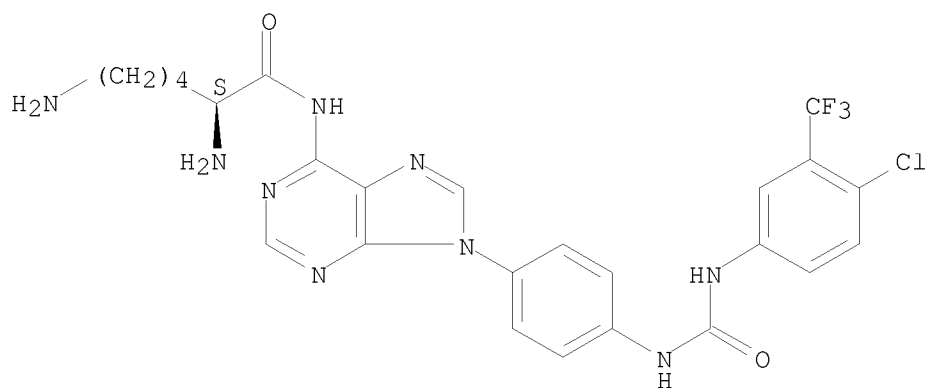
Absolute stereochemistry.



● HCl

RN 863674-11-7 CAPLUS
 CN Hexanamide, 2,6-diamino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

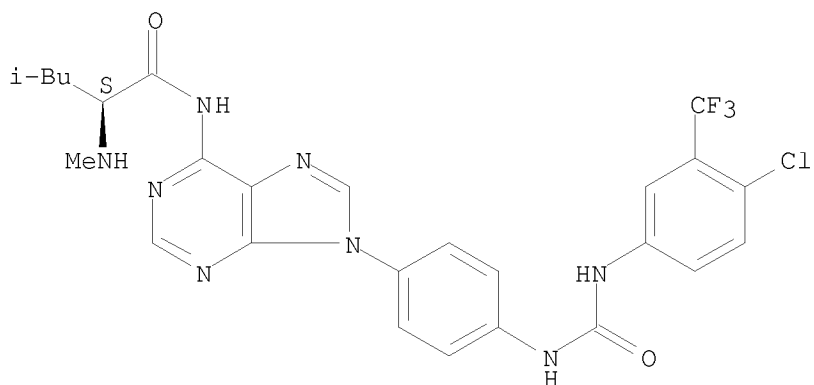
Absolute stereochemistry.



● 2 HCl

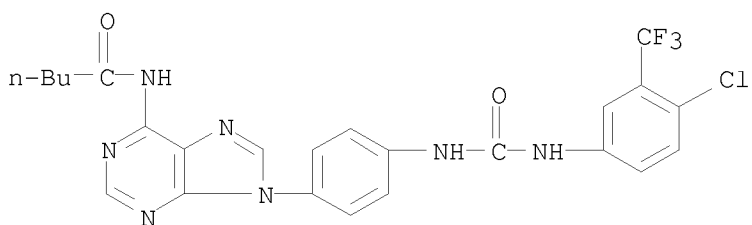
RN 863674-12-8 CAPLUS
 CN Pentanamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-4-methyl-2-(methylamino)-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

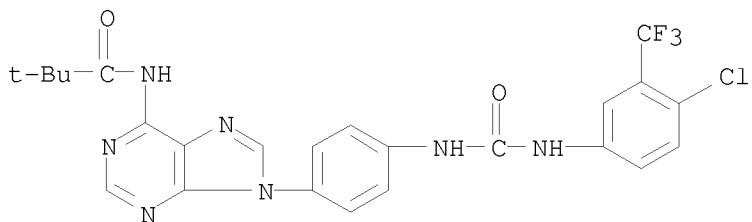


● HCl

RN 863674-13-9 CAPLUS
 CN Pentanamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]- (CA INDEX NAME)

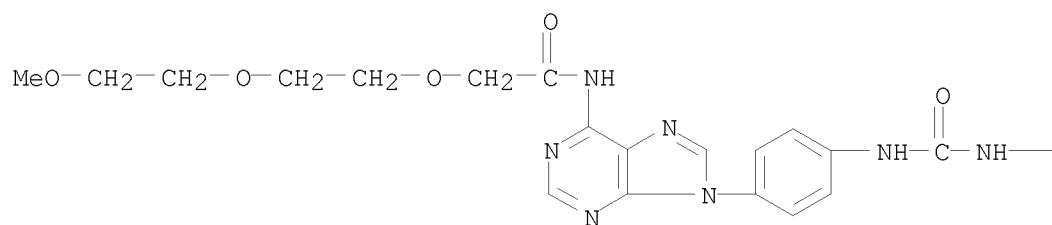


RN 863674-14-0 CAPLUS
 CN Propanamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-2,2-dimethyl- (CA INDEX NAME)

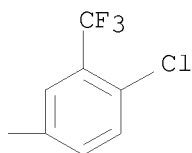


RN 863674-15-1 CAPLUS
 CN Acetamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-2-[2-(2-methoxyethoxy)ethoxy]- (CA INDEX NAME)

PAGE 1-A

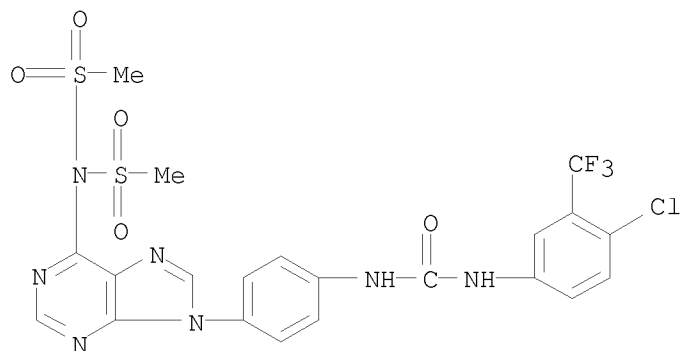


PAGE 1-B



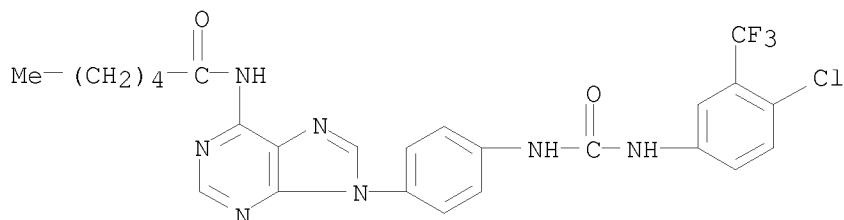
RN 863674-16-2 CAPLUS

CN Methanesulfonamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N-(methylsulfonyl)- (CA INDEX NAME)



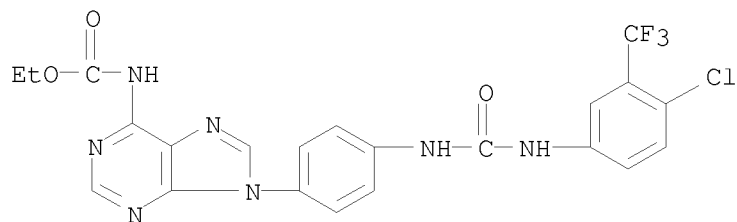
RN 863674-17-3 CAPLUS

CN Hexanamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]- (CA INDEX NAME)



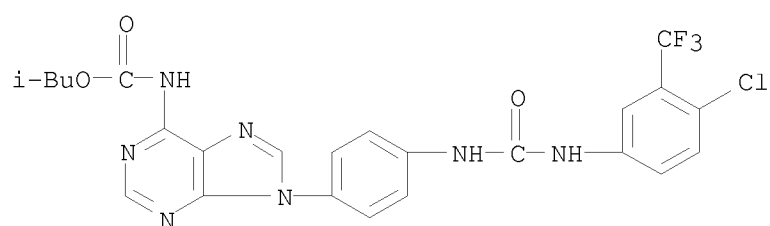
RN 863674-18-4 CAPLUS

CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, ethyl ester (9CI) (CA INDEX NAME)



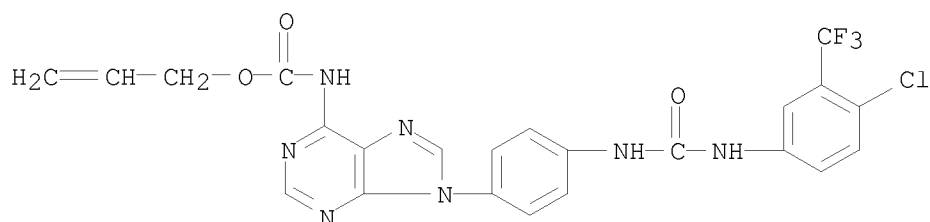
RN 863674-19-5 CAPLUS

CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



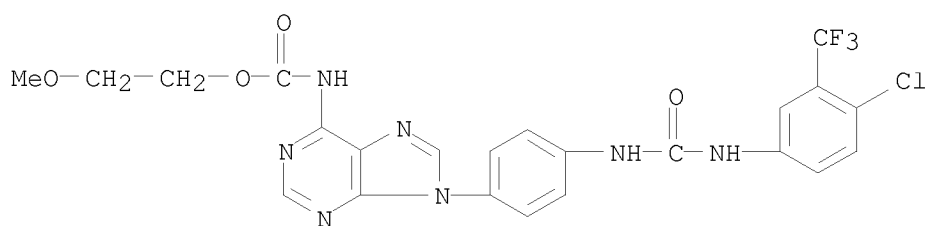
RN 863674-20-8 CAPLUS

CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-propenyl ester (9CI) (CA INDEX NAME)



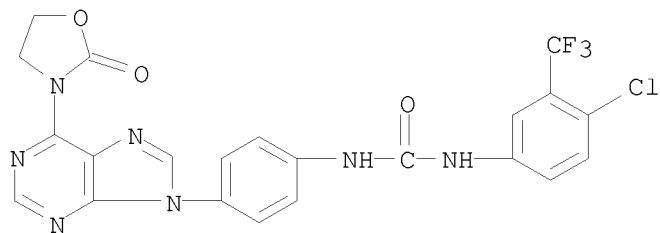
RN 863674-21-9 CAPLUS

CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-methoxyethyl ester (9CI) (CA INDEX NAME)



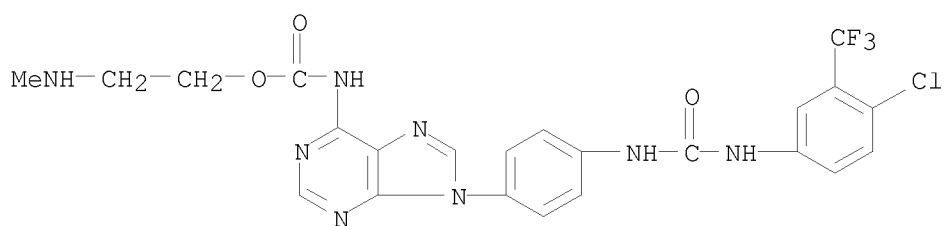
RN 863674-22-0 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(2-oxo-3-oxazolidinyl)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



RN 863674-23-1 CAPLUS

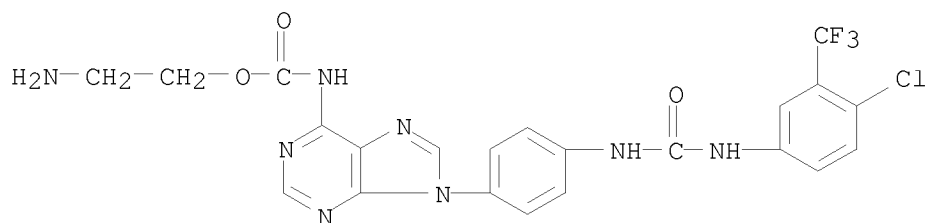
CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-(methylamino)ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 863674-24-2 CAPLUS

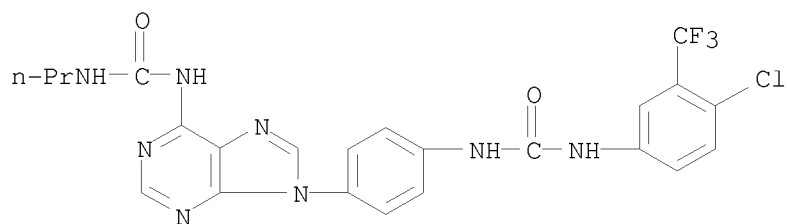
CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-aminoethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

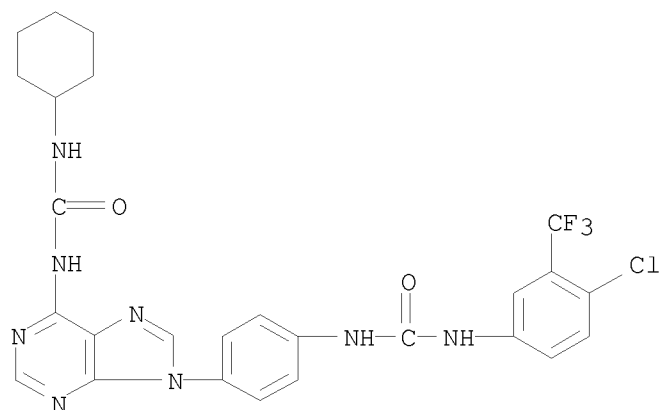
RN 863674-25-3 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-propyl- (CA INDEX NAME)



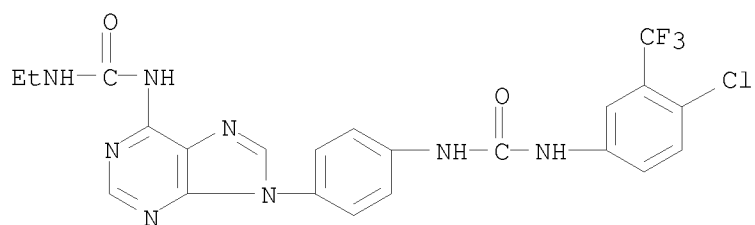
RN 863674-26-4 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-cyclohexyl- (CA INDEX NAME)



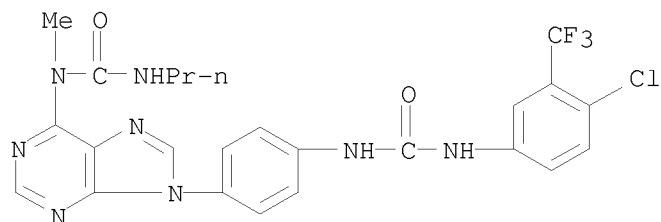
RN 863674-27-5 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-ethyl- (CA INDEX NAME)



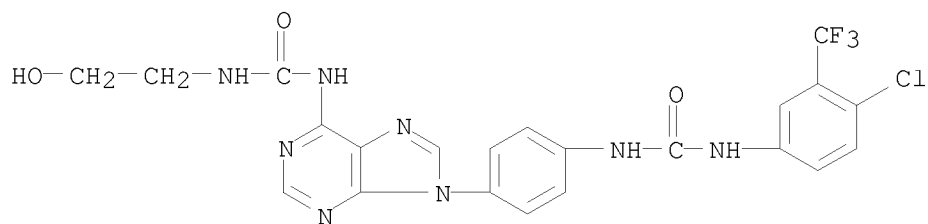
RN 863674-29-7 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N-methyl-N'-propyl- (CA INDEX NAME)



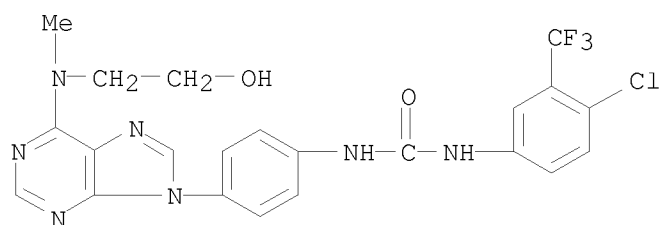
RN 863674-30-0 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-(2-hydroxyethyl)- (CA INDEX NAME)



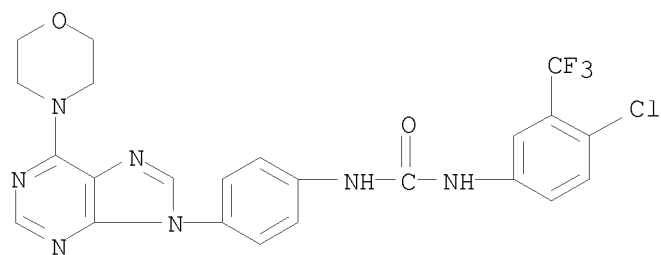
RN 863674-31-1 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-[(2-hydroxyethyl)methylamino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



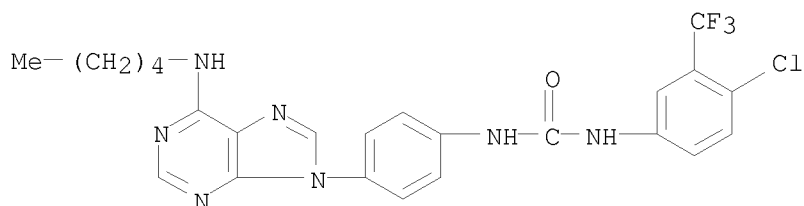
RN 863674-32-2 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(4-morpholinyl)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



RN 863674-33-3 CAPLUS

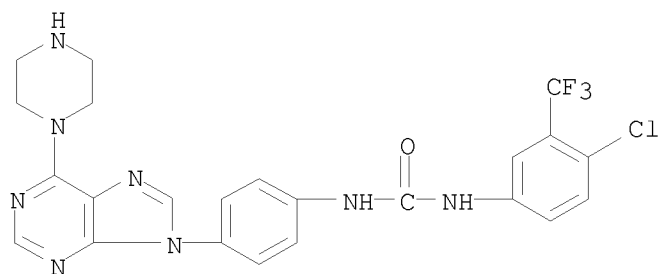
CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(pentylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



RN 863674-34-4 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(1-piperazinyl)-9H-

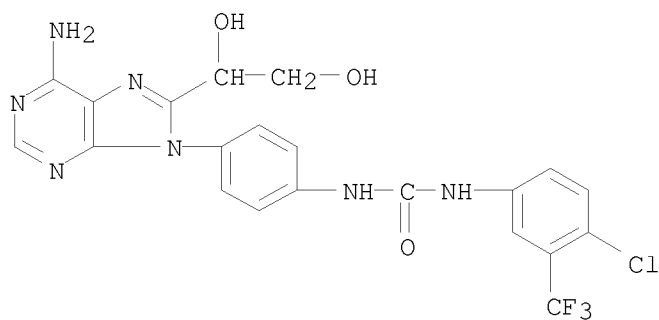
purin-9-yl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

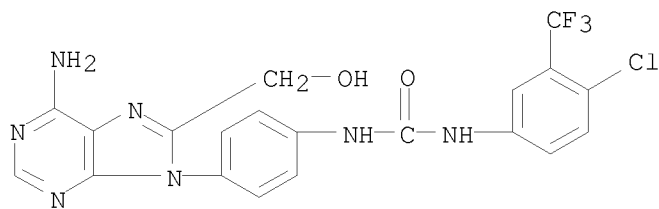
RN 863674-37-7 CAPLUS

CN Urea, N-[4-[6-amino-8-(1,2-dihydroxyethyl)-9H-purin-9-yl]phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



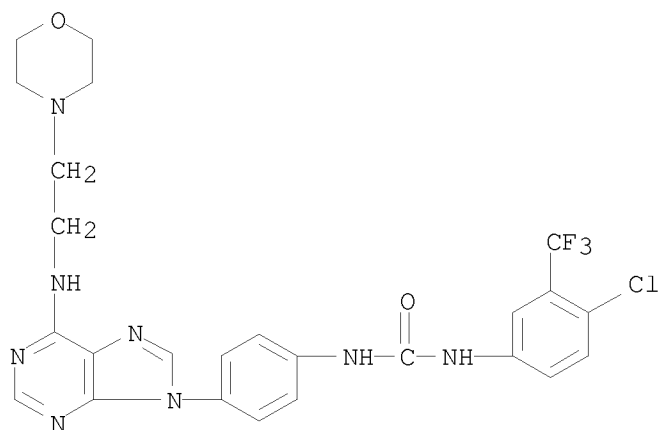
RN 863674-38-8 CAPLUS

CN Urea, N-[4-[6-amino-8-(hydroxymethyl)-9H-purin-9-yl]phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



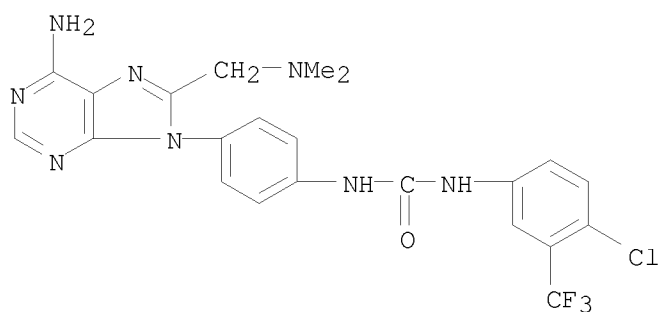
RN 863674-39-9 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-[[2-(4-morpholinyl)ethyl]amino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



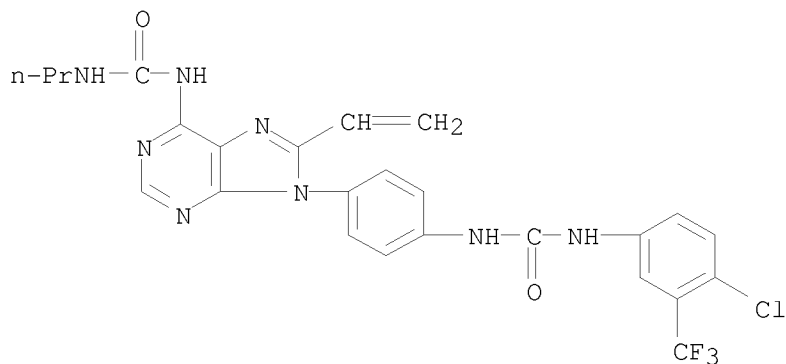
RN 863674-40-2 CAPLUS

CN Urea, N-[4-[6-amino-8-[(dimethylamino)methyl]-9H-purin-9-yl]phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



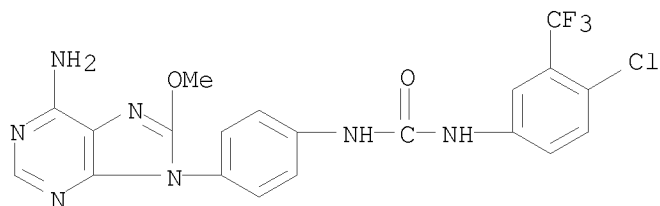
RN 863674-41-3 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-8-ethenyl-9H-purin-6-yl]-N'-propyl- (CA INDEX NAME)



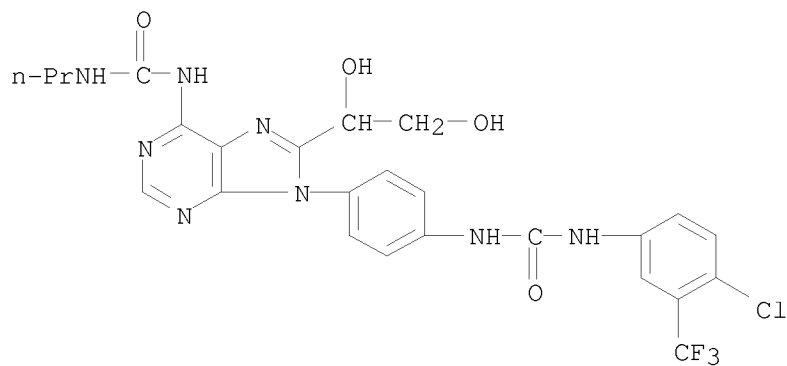
RN 863674-42-4 CAPLUS

CN Urea, N-[4-(6-amino-8-methoxy-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



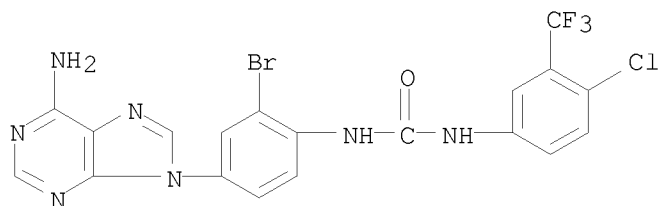
RN 863674-43-5 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-8-(1,2-dihydroxyethyl)-9H-purin-6-yl]-N'-propyl- (CA INDEX NAME)



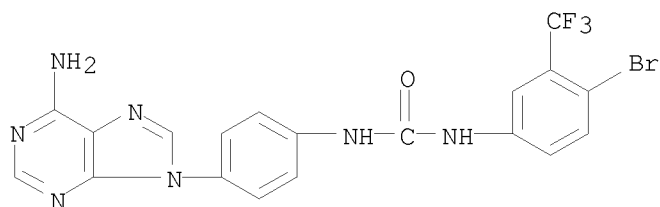
RN 863674-44-6 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)-2-bromophenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 863674-45-7 CAPLUS

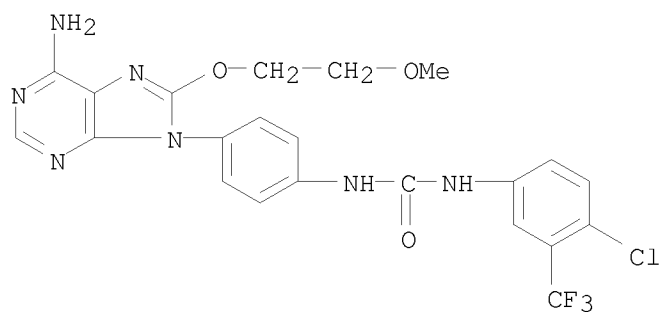
CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-bromo-3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

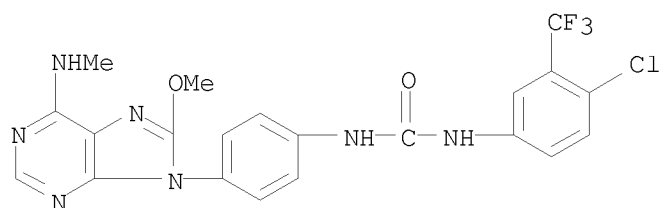
RN 863674-46-8 CAPLUS

CN Urea, N-[4-[6-amino-8-(2-methoxyethoxy)-9H-purin-9-yl]phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



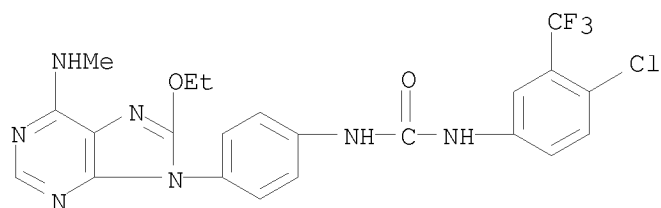
RN 863674-51-5 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-methoxy-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



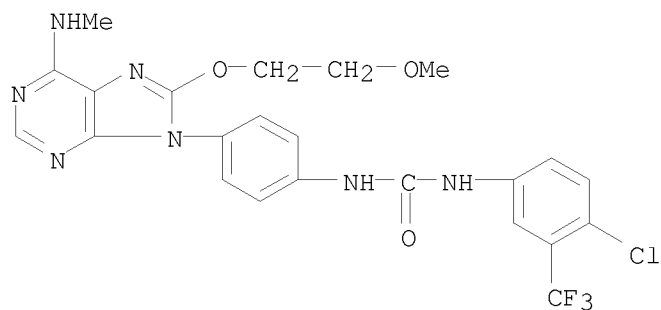
RN 863674-52-6 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-ethoxy-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



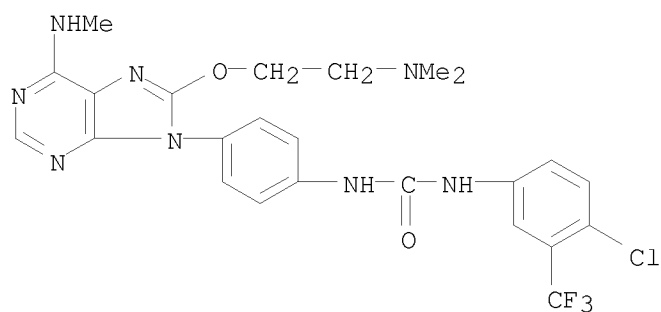
RN 863674-53-7 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-(2-methoxyethoxy)-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



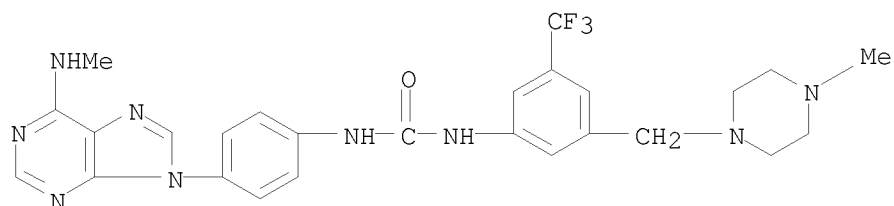
RN 863674-54-8 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-[2-(dimethylamino)ethoxy]-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



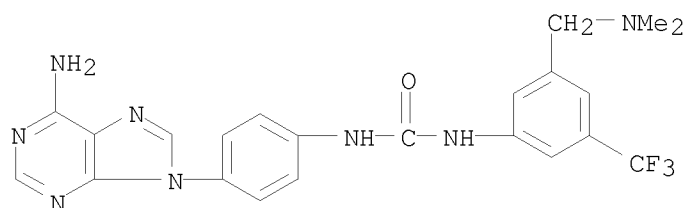
RN 863674-55-9 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



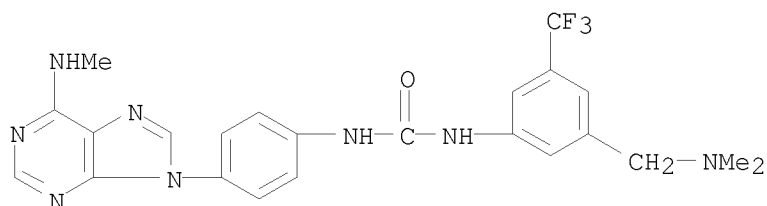
RN 863674-59-3 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-[(dimethylamino)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



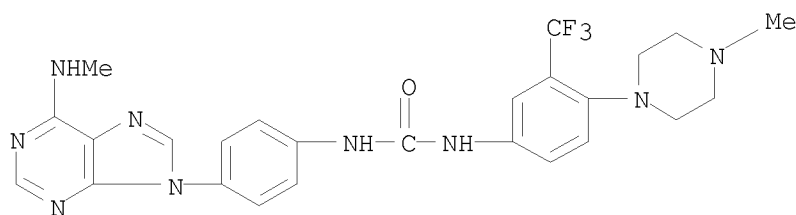
RN 863674-60-6 CAPLUS

CN Urea, N-[3-[(dimethylamino)methyl]-5-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



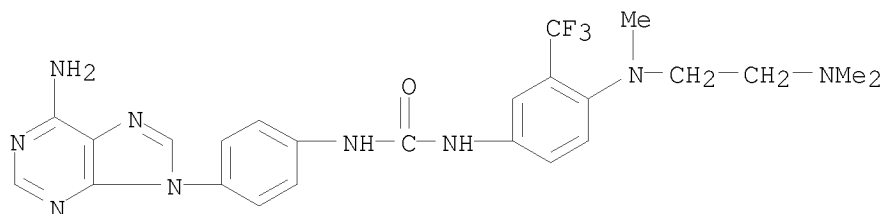
RN 863674-65-1 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(4-methyl-1-piperazinyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



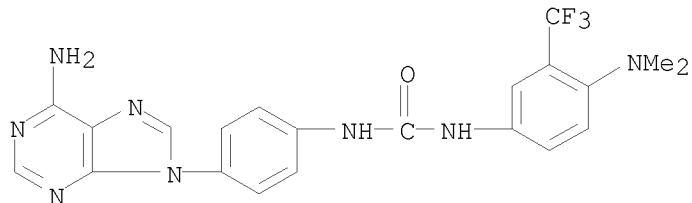
RN 863674-66-2 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-[[2-(dimethylamino)ethyl]methylamino]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



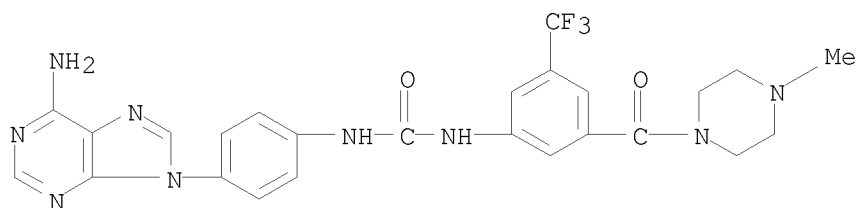
RN 863674-67-3 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-(dimethylamino)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



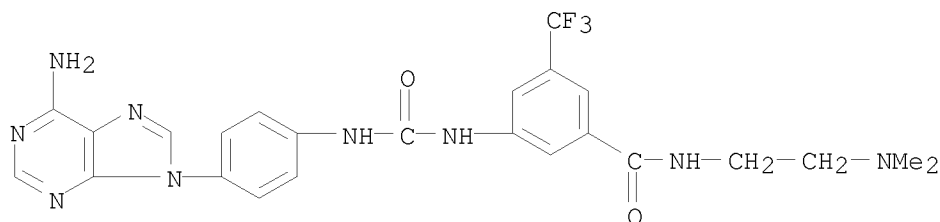
RN 863674-68-4 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)carbonyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



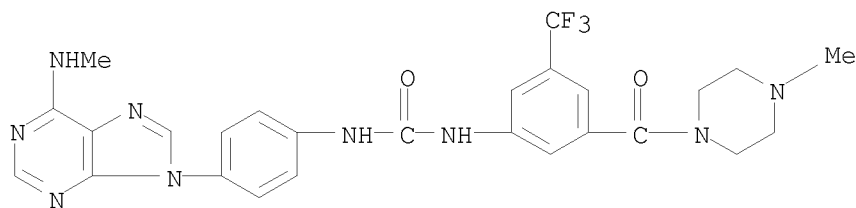
RN 863674-69-5 CAPLUS

CN Benzamide, 3-[[[4-(6-amino-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-N-[2-(dimethylamino)ethyl]-5-(trifluoromethyl)- (CA INDEX NAME)



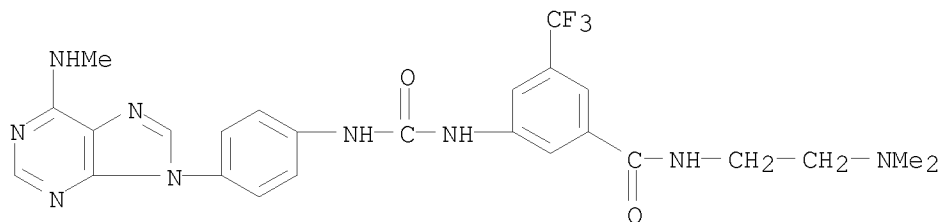
RN 863674-70-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[(4-methyl-1-piperazinyl)carbonyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



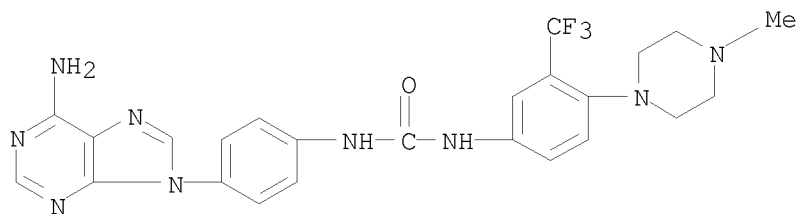
RN 863674-71-9 CAPLUS

CN Benzamide, N-[2-(dimethylamino)ethyl]-3-[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)



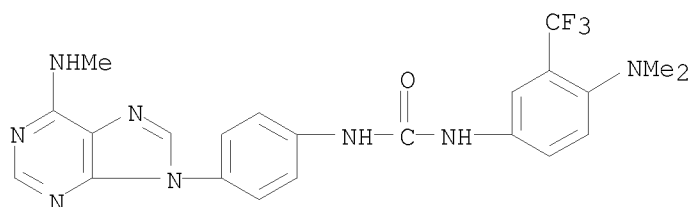
RN 863674-72-0 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-(4-methyl-1-piperazinyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



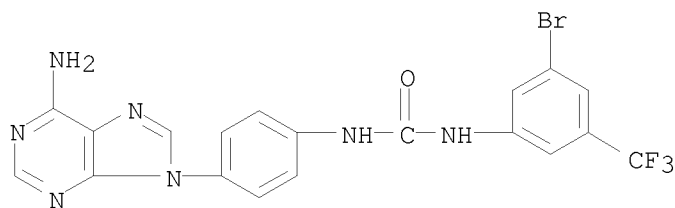
RN 863674-73-1 CAPLUS

CN Urea, N-[4-(dimethylamino)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



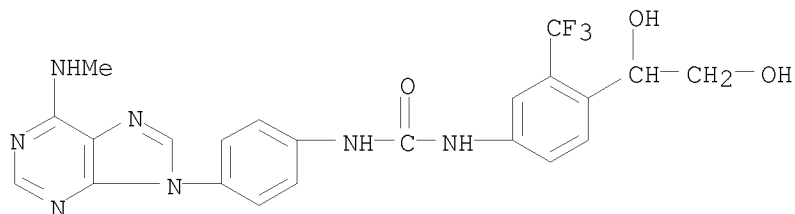
RN 863674-74-2 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-bromo-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



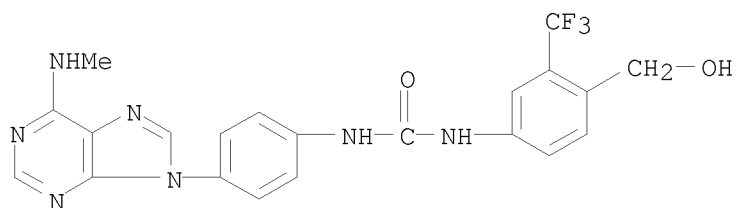
RN 863674-75-3 CAPLUS

CN Urea, N-[4-(1,2-dihydroxyethyl)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



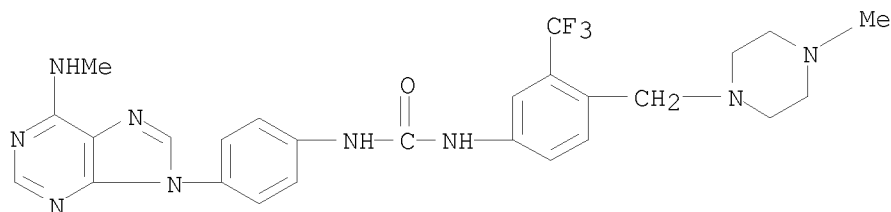
RN 863674-76-4 CAPLUS

CN Urea, N-[4-(hydroxymethyl)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



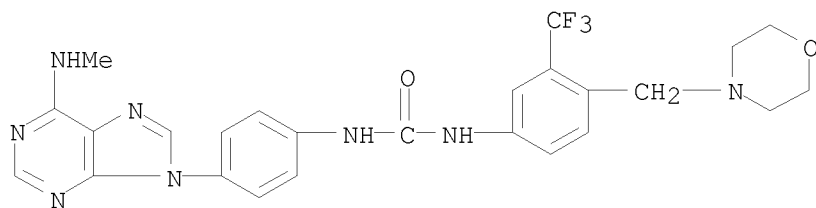
RN 863674-77-5 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[(4-methyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



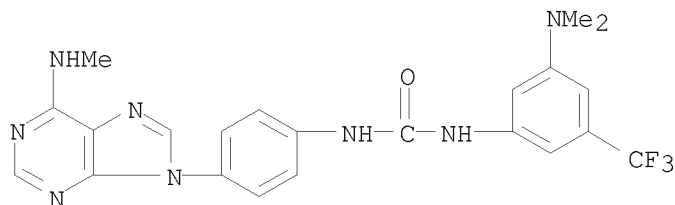
RN 863674-78-6 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(4-morpholinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



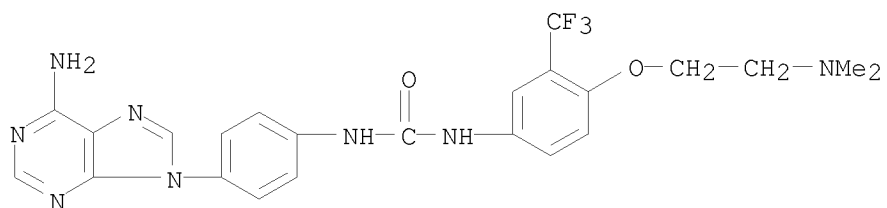
RN 863674-79-7 CAPLUS

CN Urea, N-[3-(dimethylamino)-5-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



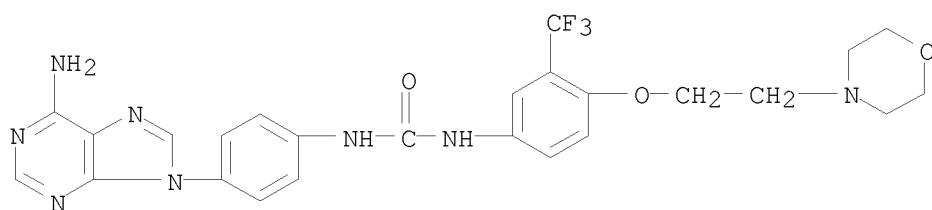
RN 863674-80-0 CAPLUS

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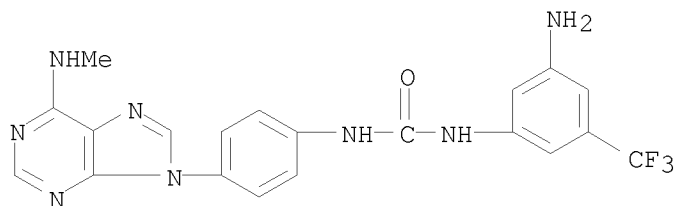
RN 863674-81-1 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-[2-(4-morpholinyl)ethoxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



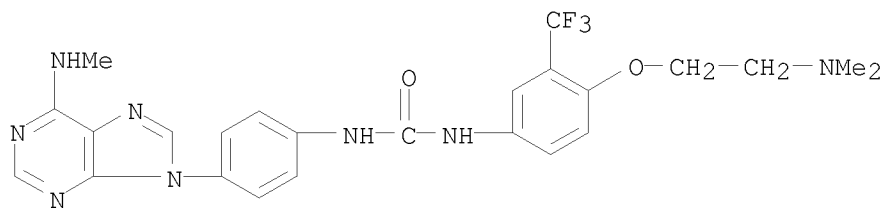
RN 863674-82-2 CAPLUS

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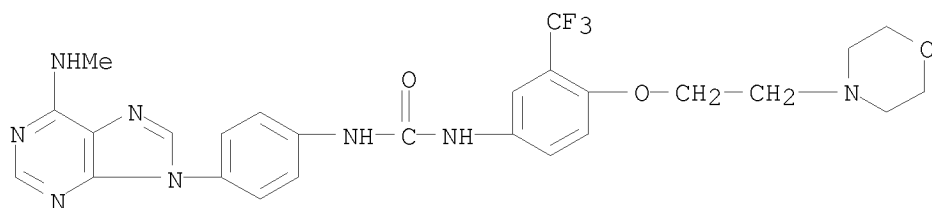
RN 863674-83-3 CAPLUS

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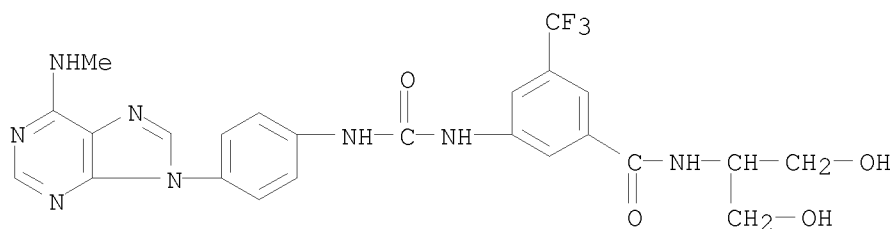
RN 863674-84-4 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(4-morpholinyl)ethoxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



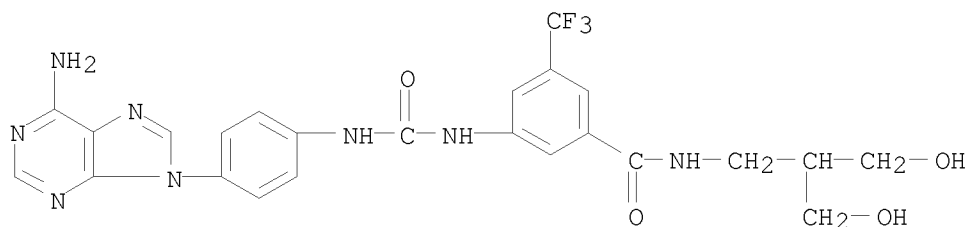
RN 863674-85-5 CAPLUS

CN Benzamide, N-[2-hydroxy-1-(hydroxymethyl)ethyl]-3-[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)



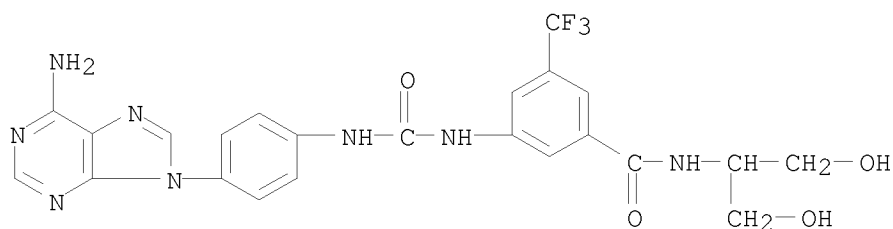
RN 863674-86-6 CAPLUS

CN Benzamide, 3-[[[4-(6-amino-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-N-[3-hydroxy-2-(hydroxymethyl)propyl]-5-(trifluoromethyl)- (CA INDEX NAME)



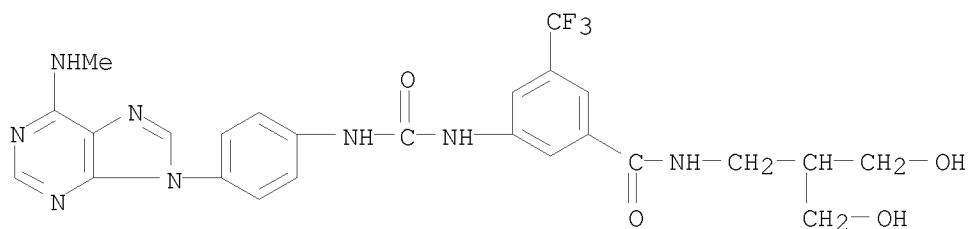
RN 863674-87-7 CAPLUS

CN Benzamide, 3-[[[4-(6-amino-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-N-[2-hydroxy-1-(hydroxymethyl)ethyl]-5-(trifluoromethyl)- (CA INDEX NAME)



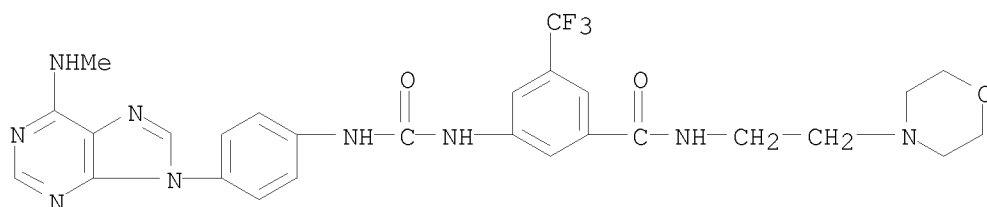
RN 863674-88-8 CAPLUS

CN Benzamide, N-[3-hydroxy-2-(hydroxymethyl)propyl]-3-[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)



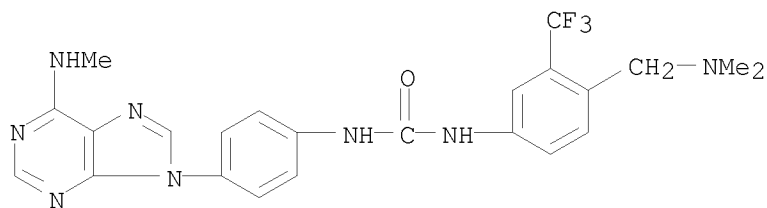
RN 863674-89-9 CAPLUS

CN Benzamide, 3-[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-N-[2-(4-morpholinyl)ethyl]-5-(trifluoromethyl)- (CA INDEX NAME)



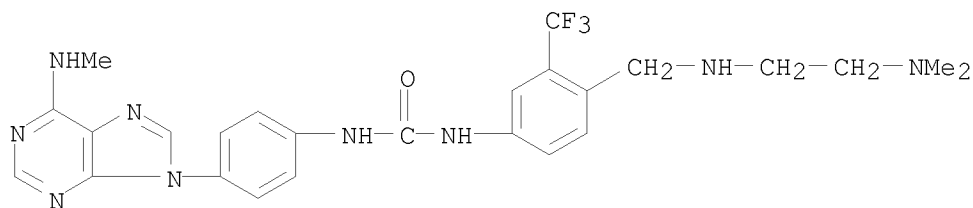
RN 863674-90-2 CAPLUS

CN Urea, N-[4-[(dimethylamino)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



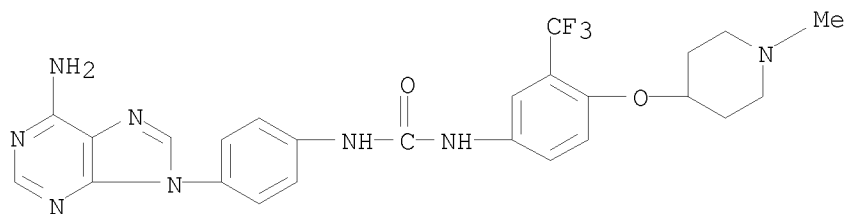
RN 863674-91-3 CAPLUS

CN Urea, N-[4-[[2-(dimethylamino)ethyl]amino]methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



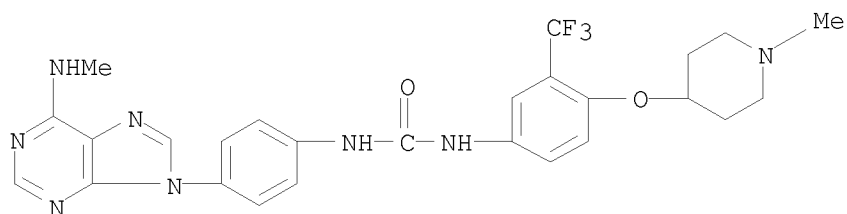
RN 863674-92-4 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-[(1-methyl-4-piperidinyl)oxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



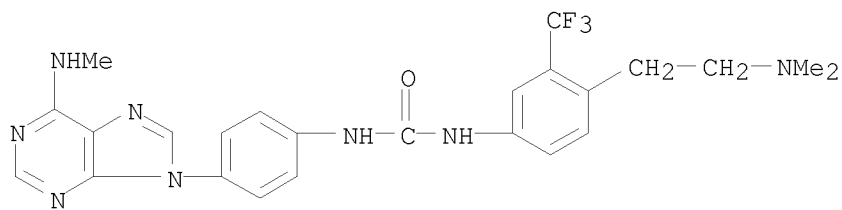
RN 863674-93-5 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[(1-methyl-4-piperidinyl)oxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



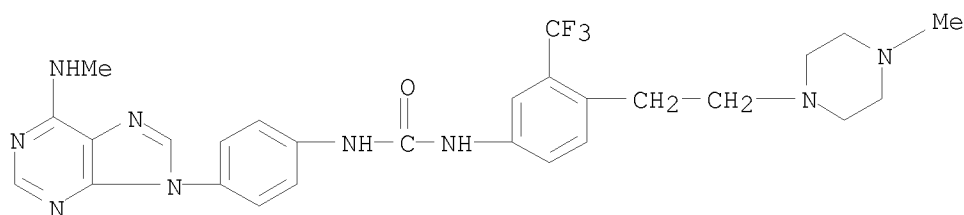
RN 863674-94-6 CAPLUS

CN Urea, N-[4-[2-(dimethylamino)ethyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



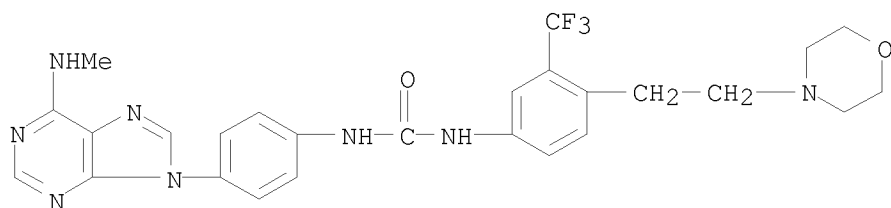
RN 863674-95-7 CAPLUS

CN Urea, N-[4-[2-(4-methyl-1-piperazinyl)ethyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



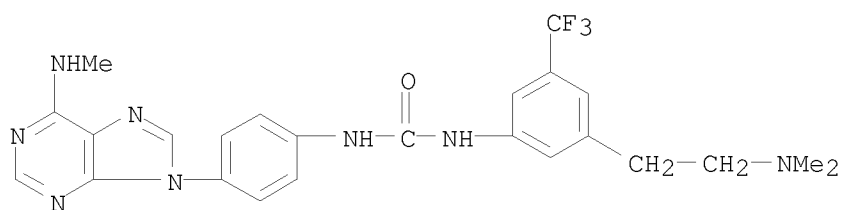
RN 863674-96-8 CAPLUS

CN Urea, N-[4-[2-(4-morpholinyl)ethyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



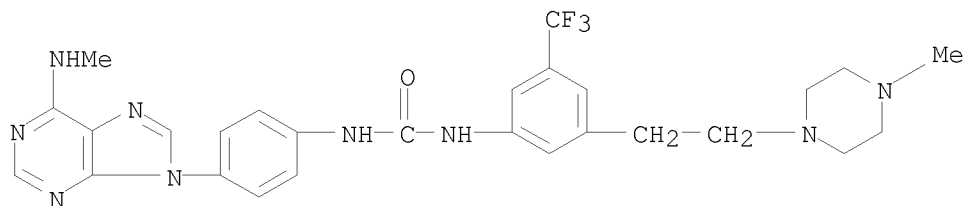
RN 863674-97-9 CAPLUS

CN Urea, N-[3-[2-(dimethylamino)ethyl]-5-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



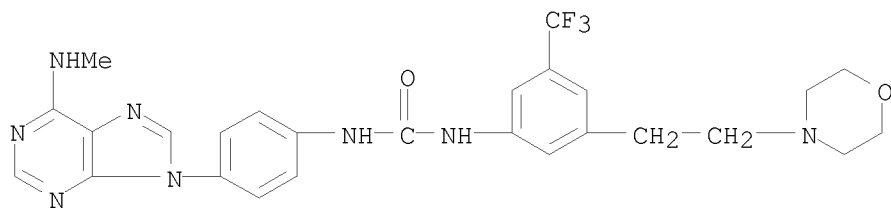
RN 863674-98-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[2-(4-methyl-1-piperazinyl)ethyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



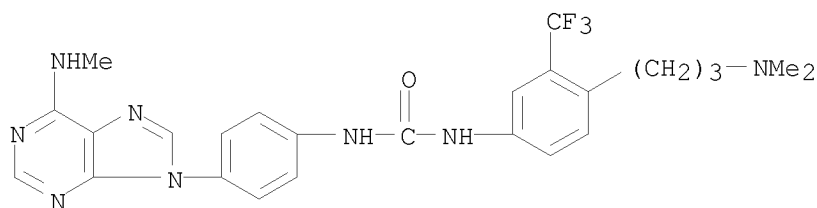
RN 863674-99-1 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[2-(4-morpholinyl)ethyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



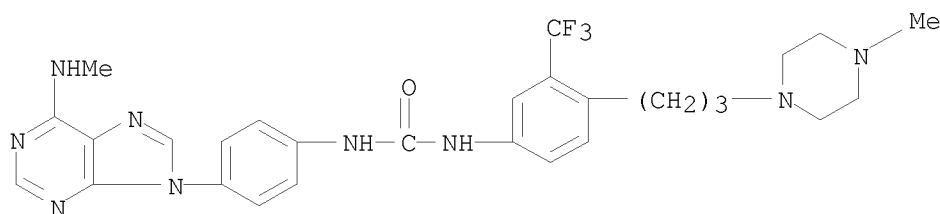
RN 863675-00-7 CAPLUS

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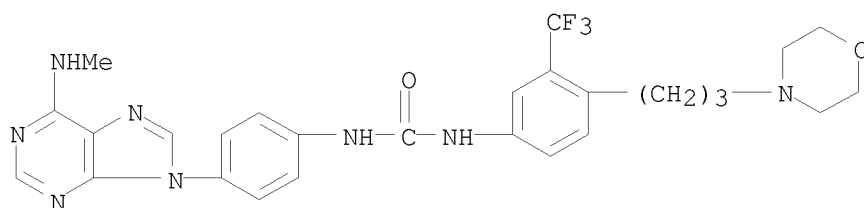
RN 863675-01-8 CAPLUS

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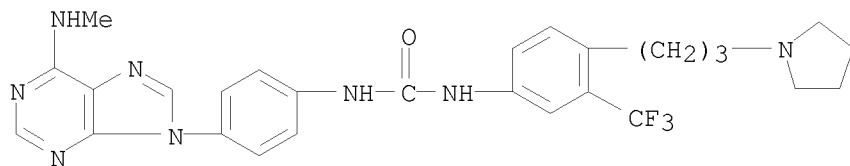
RN 863675-02-9 CAPLUS

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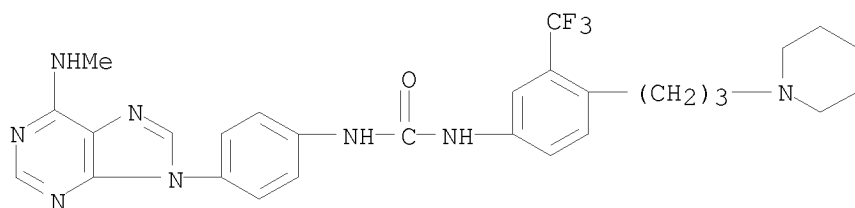
RN 863675-03-0 CAPLUS

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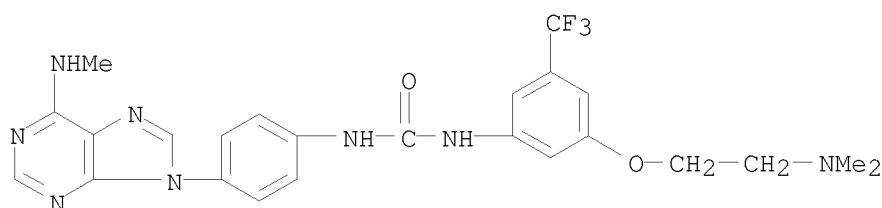
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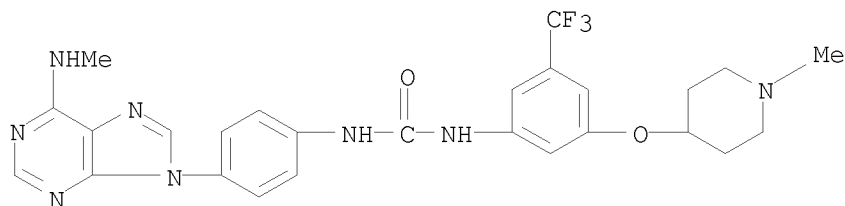
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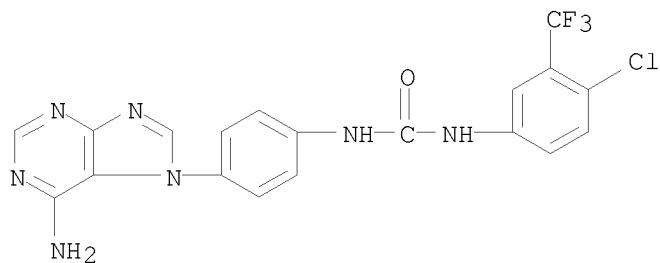
RN 863675-06-3 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[(1-methyl-4-piperidinyl)oxy]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 863675-07-4 CAPLUS

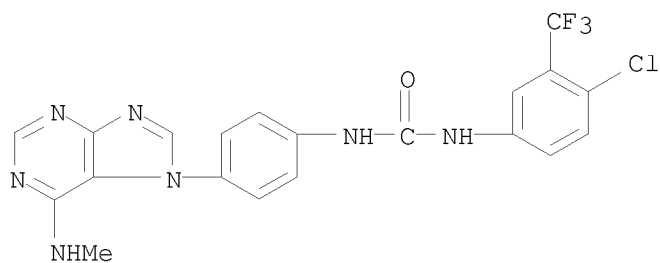
CN Urea, N-[4-(6-amino-7H-purin-7-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 863675-08-5 CAPLUS

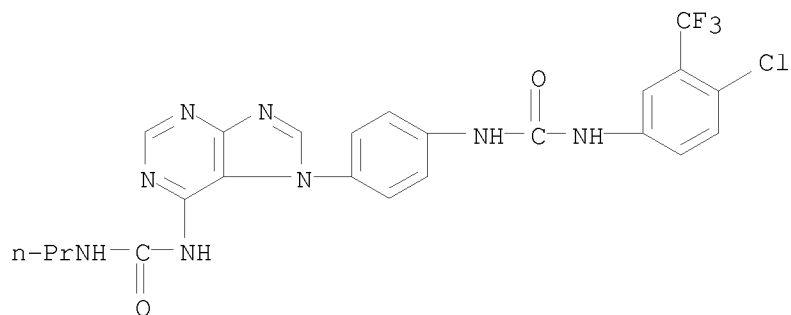
CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-7H-purin-7-yl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

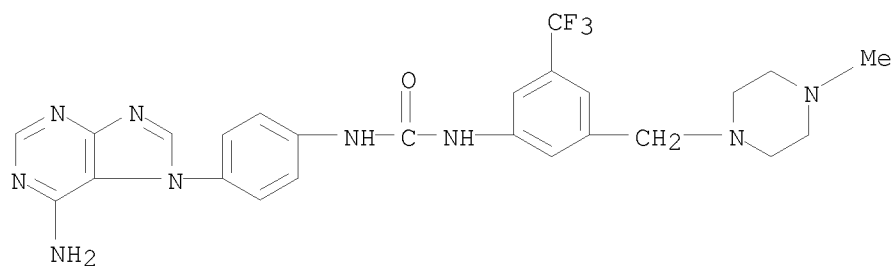
RN 863675-09-6 CAPLUS

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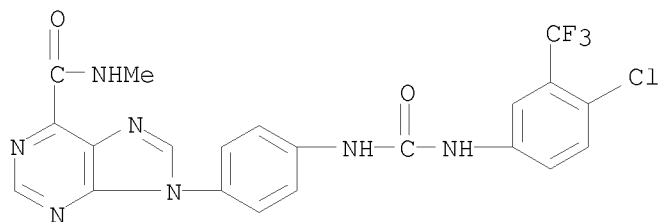
RN 863675-10-9 CAPLUS

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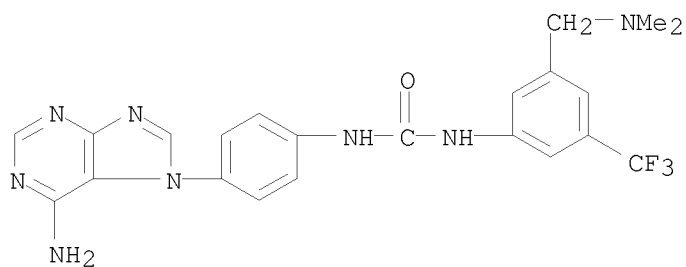
RN 863675-13-2 CAPLUS

CN 9H-Purine-6-carboxamide, 9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-N-methyl- (CA INDEX NAME)



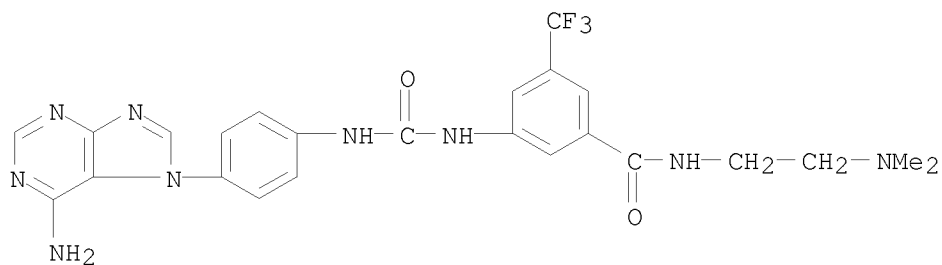
RN 863675-14-3 CAPLUS

CN Urea, N-[4-(6-amino-7H-purin-7-yl)phenyl]-N'-[3-[(dimethylamino)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



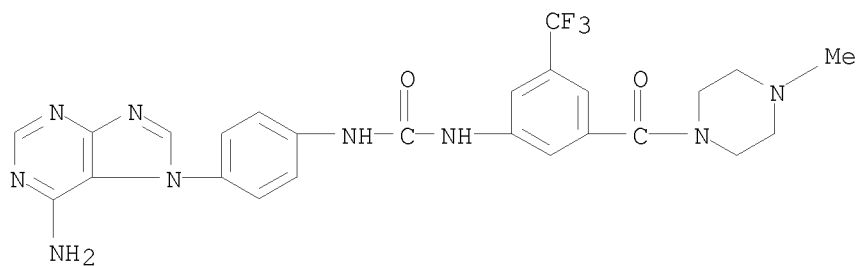
RN 863675-15-4 CAPLUS

CN Benzamide, 3-[[[4-(6-amino-7H-purin-7-yl)phenyl]amino]carbonyl]amino]-N-[2-(dimethylamino)ethyl]-5-(trifluoromethyl)- (CA INDEX NAME)



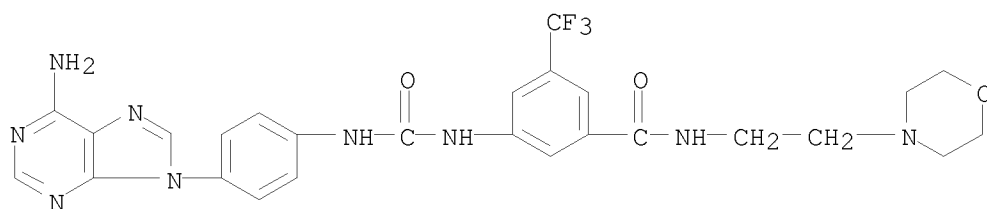
RN 863675-16-5 CAPLUS

CN Urea, N-[4-(6-amino-7H-purin-7-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)carbonyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



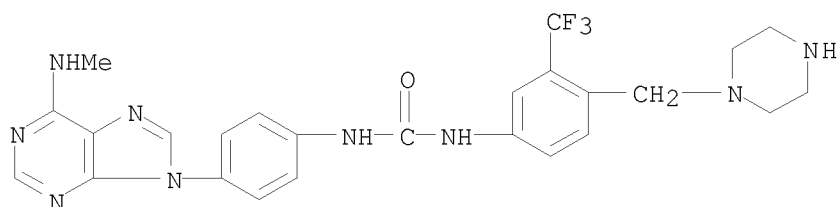
RN 863675-17-6 CAPLUS

CN Benzamide, 3-[[[4-(6-amino-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-N-[2-(4-morpholinyl)ethyl]-5-(trifluoromethyl)- (CA INDEX NAME)



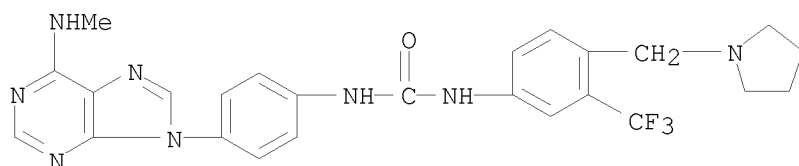
RN 863675-18-7 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(1-piperazinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



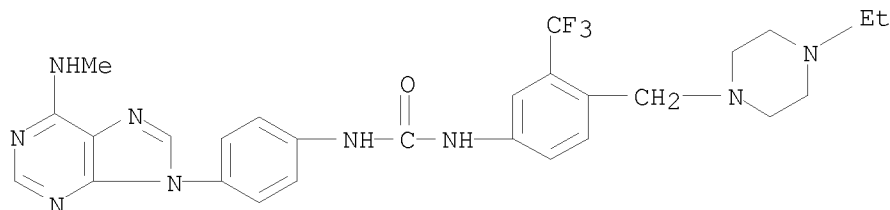
RN 863675-19-8 CAPLUS

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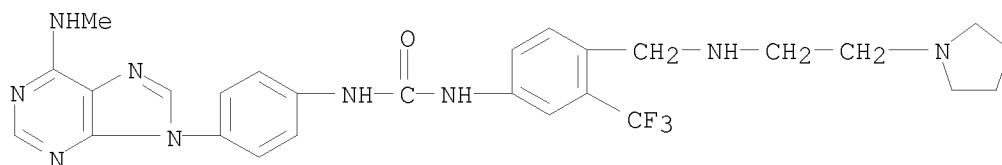
RN 863675-20-1 CAPLUS

CN Urea, N-[4-[4-ethyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



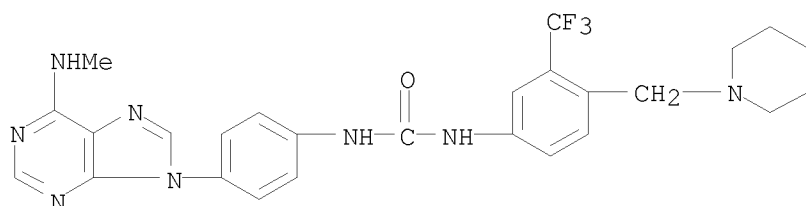
RN 863675-21-2 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[[2-(1-pyrrolidinyl)ethyl]amino]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



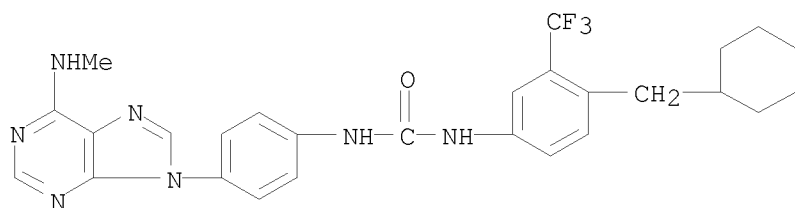
RN 863675-22-3 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(1-piperidinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



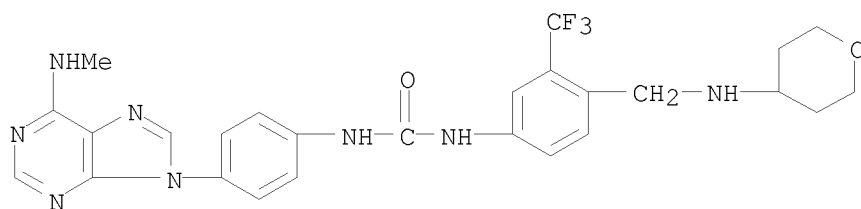
RN 863675-23-4 CAPLUS

CN Urea, N-[4-(cyclohexylmethyl)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



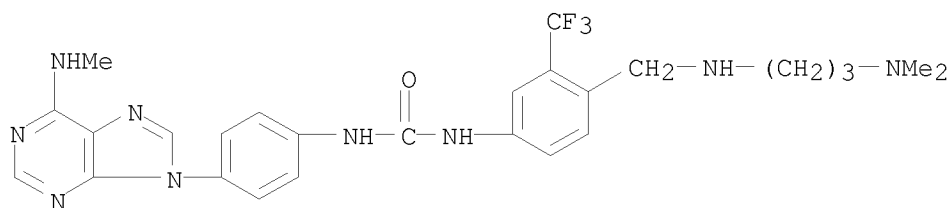
RN 863675-25-6 CAPLUS

CN Urea, N-[4-[[3-(dimethylamino)propyl]amino]methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



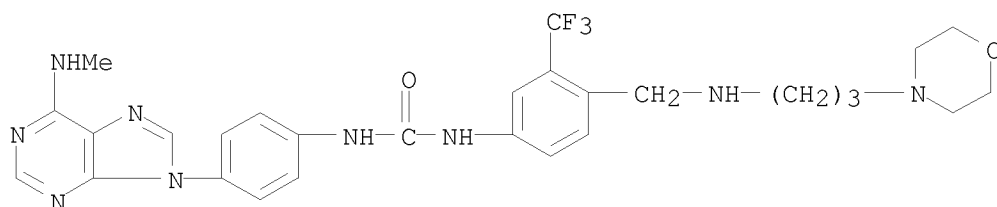
RN 863675-26-7 CAPLUS

CN Urea, N-[4-[[3-(dimethylamino)propyl]amino]methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



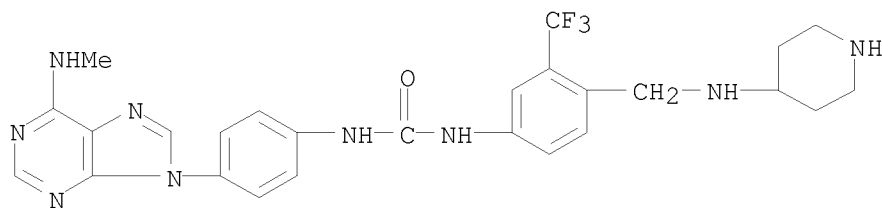
RN 863675-27-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[[3-(4-morpholinyl)propyl]amino]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



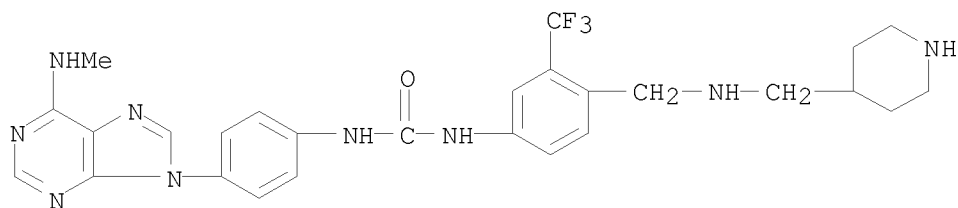
RN 863675-28-9 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[(4-piperidinylamino)methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



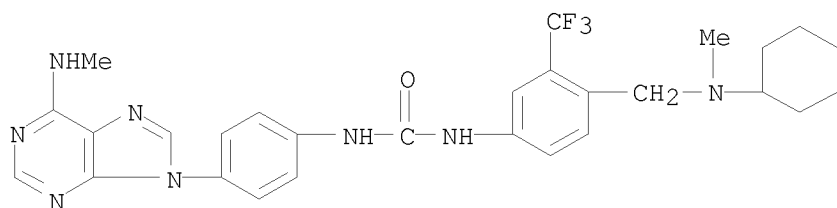
RN 863675-29-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[[4-(piperidinylmethyl)amino]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



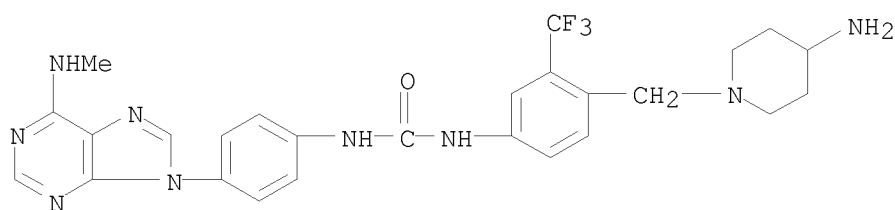
RN 863675-30-3 CAPLUS

CN Urea, N-[4-[(cyclohexylmethylamino)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



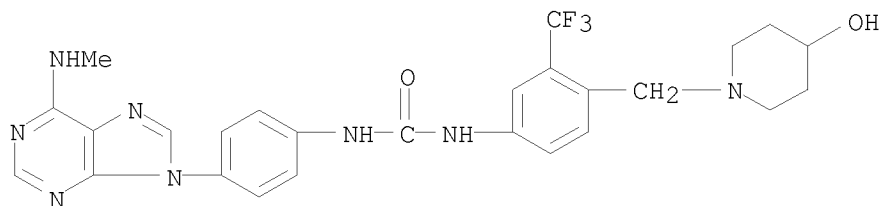
RN 863675-31-4 CAPLUS

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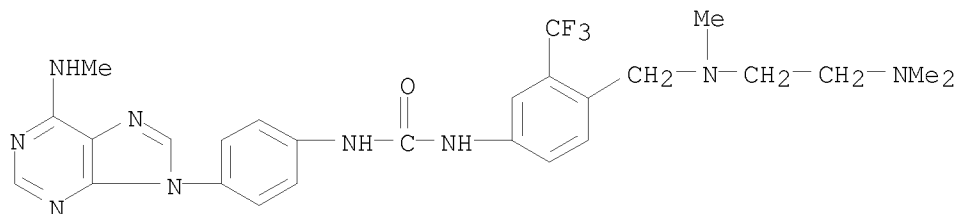
RN 863675-32-5 CAPLUS

CN Urea, N-[4-[(4-hydroxy-1-piperidinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



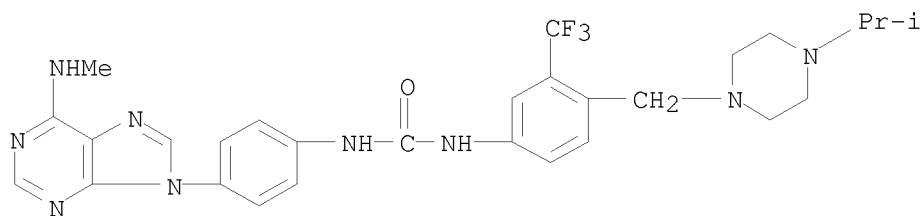
RN 863675-33-6 CAPLUS

CN Urea, N-[4-[[[2-(dimethylamino)ethyl]methylamino]methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



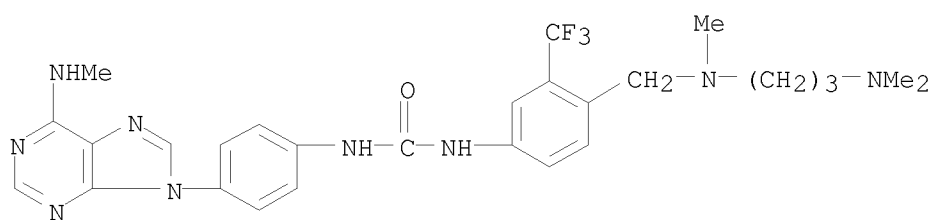
RN 863675-34-7 CAPLUS

CN Urea, N-[4-[(4-(1-methylethyl)-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



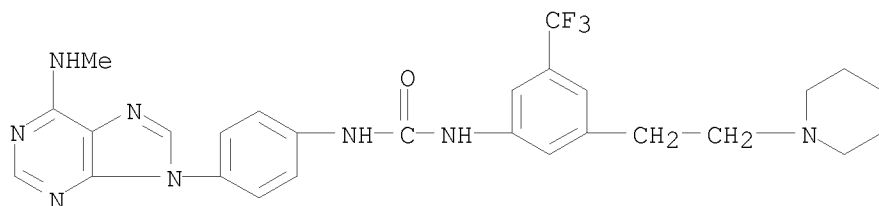
RN 863675-35-8 CAPLUS

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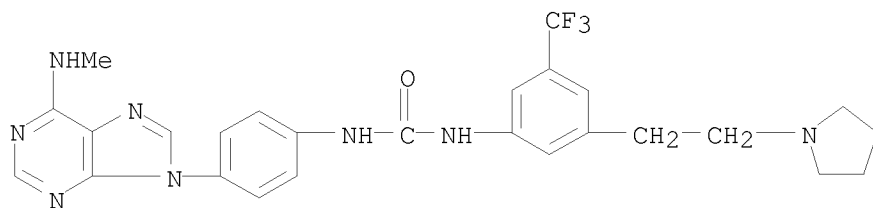
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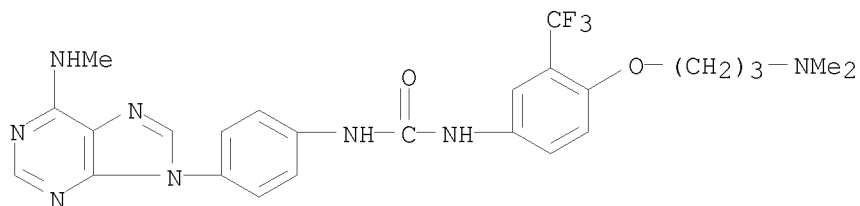
RN 863675-37-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[2-(1-pyrrolidiny)ethyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



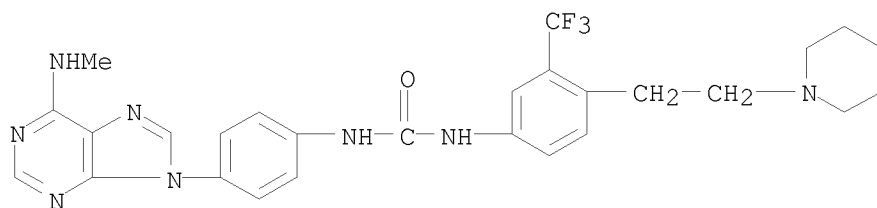
RN 863675-38-1 CAPLUS

CN Urea, N-[4-[3-(dimethylamino)propoxy]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



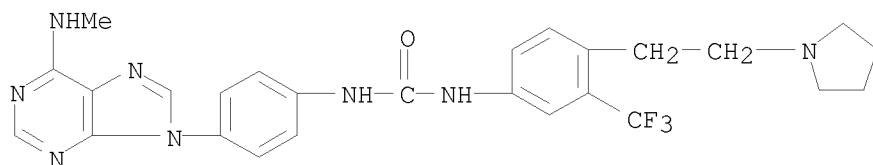
RN 863675-39-2 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(1-piperidinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



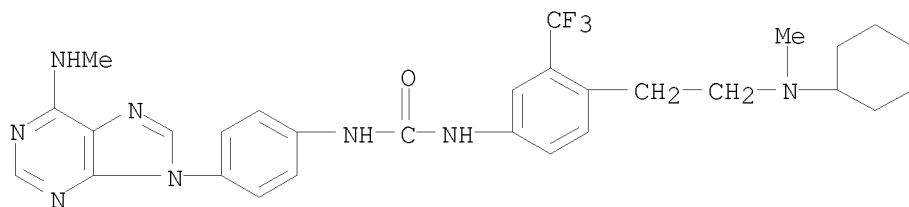
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CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(1-pyrrolidinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



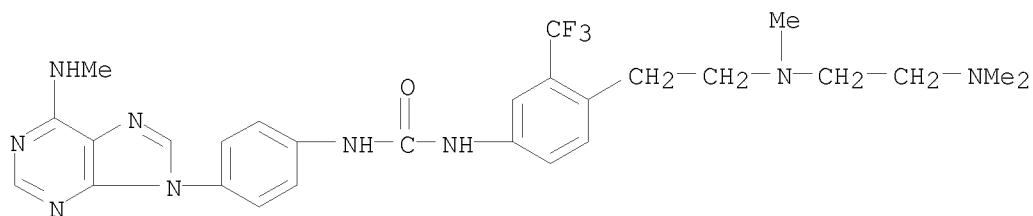
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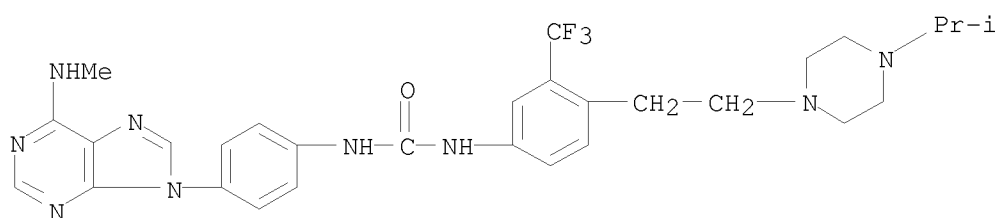
RN 863675-42-7 CAPLUS

CN Urea, N-[4-[2-[[2-(dimethylamino)ethyl]methylamino]ethyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



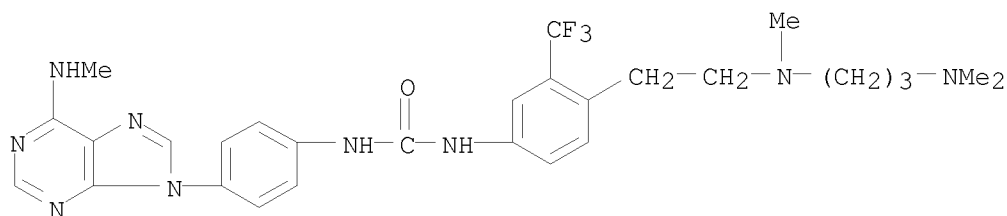
RN 863675-43-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-[4-(1-methylethyl)-1-piperazinyl]ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



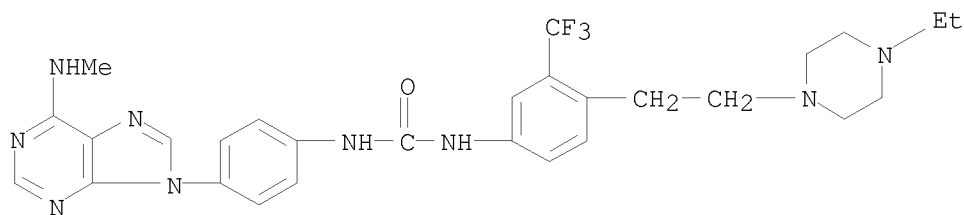
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CN Urea, N-[4-[2-[3-(dimethylamino)propyl]methylamino]ethyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



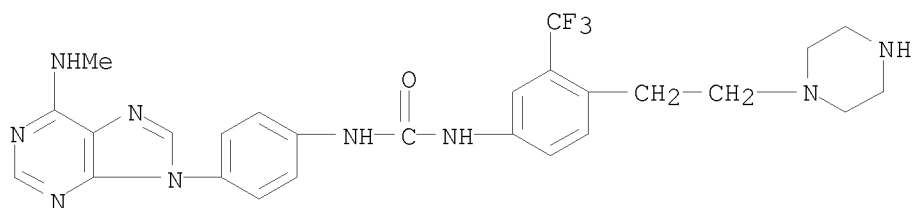
RN 863675-45-0 CAPLUS

CN Urea, N-[4-[2-(4-ethyl-1-piperazinyl)ethyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



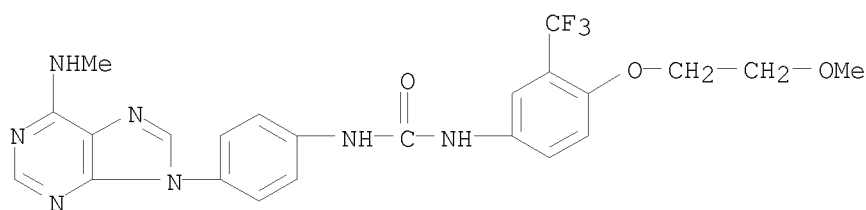
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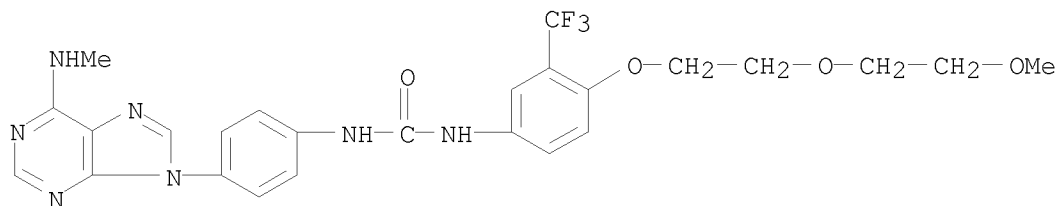
RN 863675-47-2 CAPLUS

CN Urea, N-[4-(2-methoxyethoxy)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



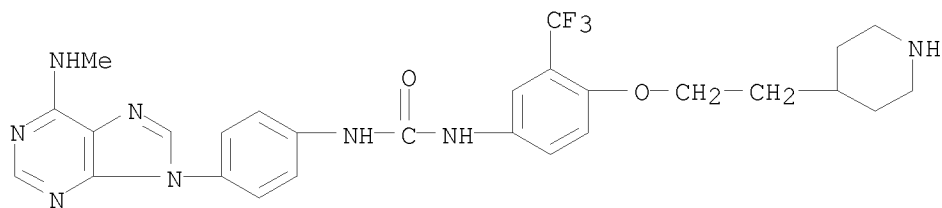
RN 863675-48-3 CAPLUS

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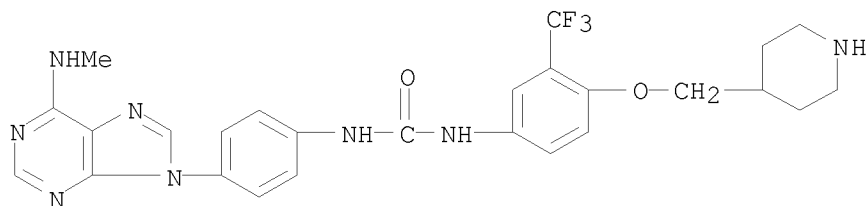
RN 863675-49-4 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(4-piperidinyl)ethoxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



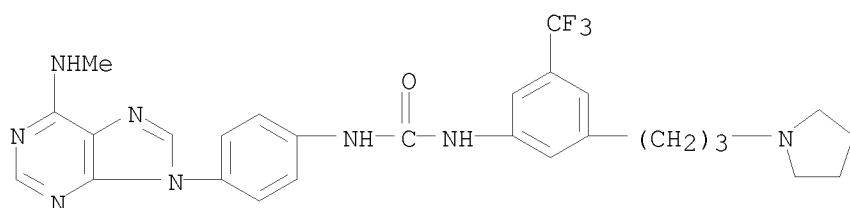
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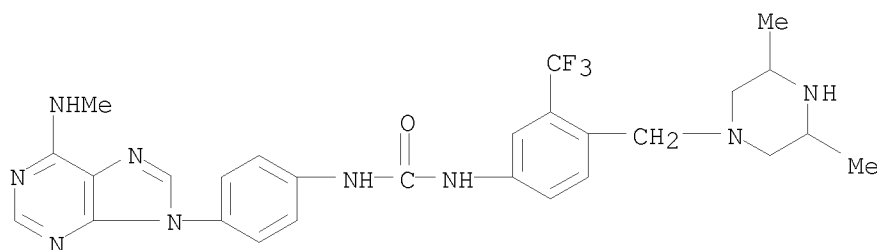
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CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[3-(1-pyrrolidinyl)propyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



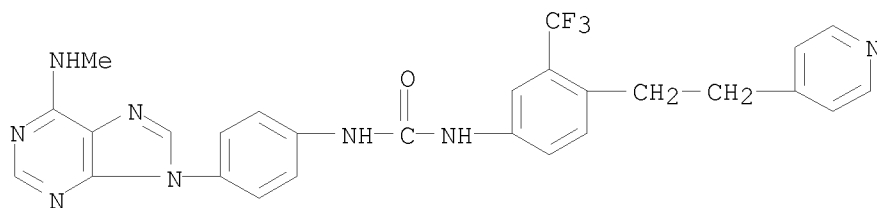
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CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[3-(1-pyrrolidinyl)propyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



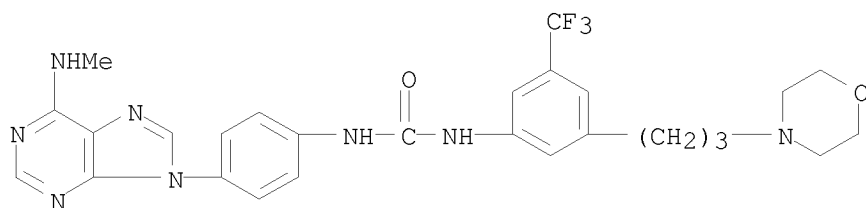
RN 863675-53-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(4-pyridinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



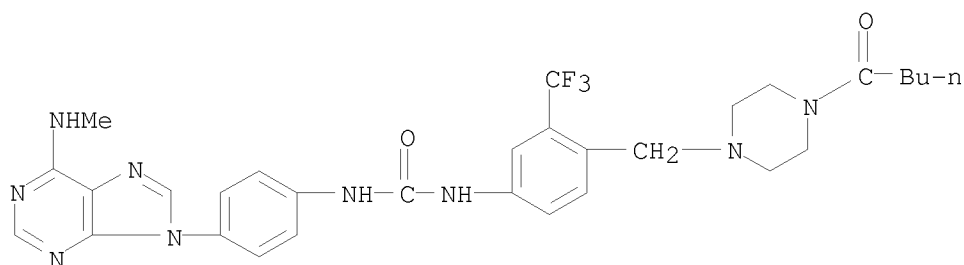
RN 863675-54-1 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[3-(4-morpholinyl)propyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



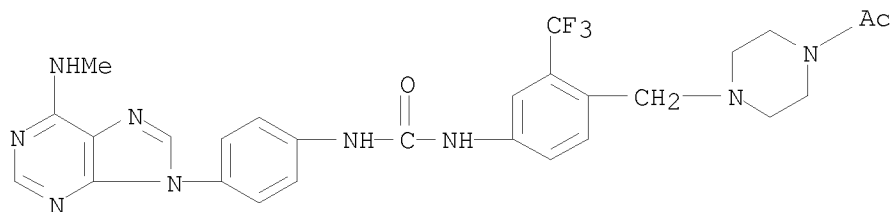
RN 863675-55-2 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[4-(1-oxopentyl)-1-piperazinyl]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



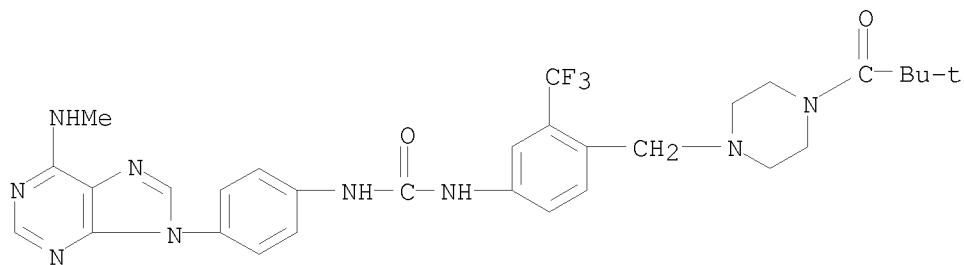
RN 863675-56-3 CAPLUS

CN Urea, N-[4-[[4-(4-acetyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



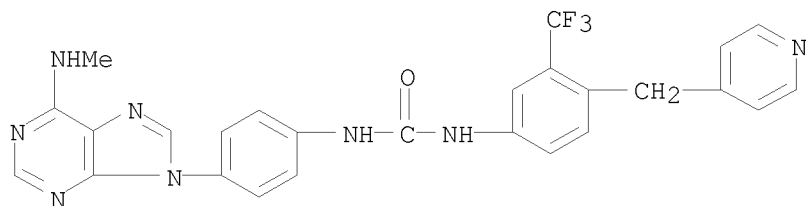
RN 863675-57-4 CAPLUS

CN Urea, N-[4-[[4-(2,2-dimethyl-1-oxopropyl)-1-piperazinyl]methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



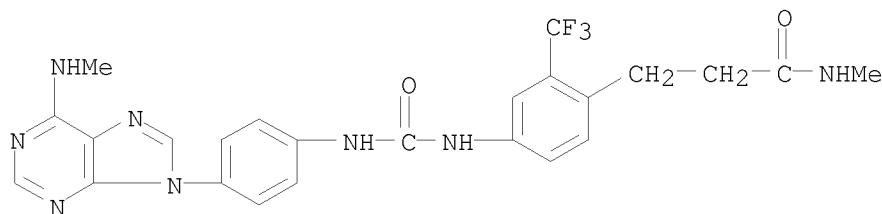
RN 863675-58-5 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(4-pyridinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 863675-59-6 CAPLUS

CN Benzenepropanamide, N-methyl-4-[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)



IT 863675-80-3P 863675-81-4P 863675-82-5P

863675-83-6P 863675-90-5P 863675-93-8P

863675-94-9P 863675-95-0P 863675-96-1P

863675-97-2P 863676-01-1P 863676-02-2P

863676-03-3P 863676-06-6P 863676-07-7P

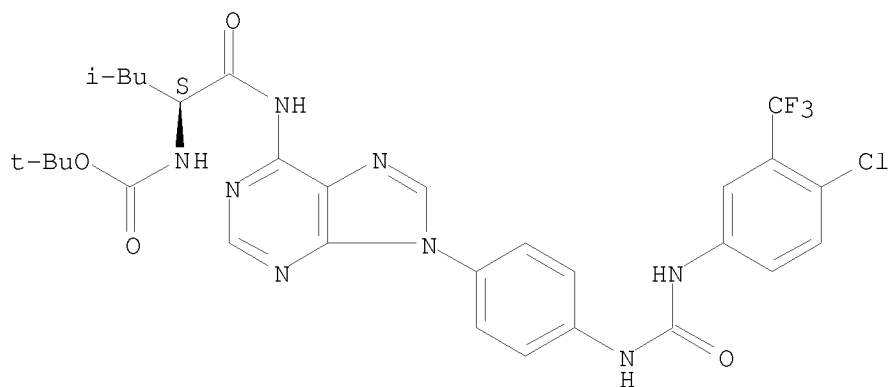
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroarylphenylurea derivs. as Raf inhibitors for treatment of cancer and diabetes)

RN 863675-80-3 CAPLUS

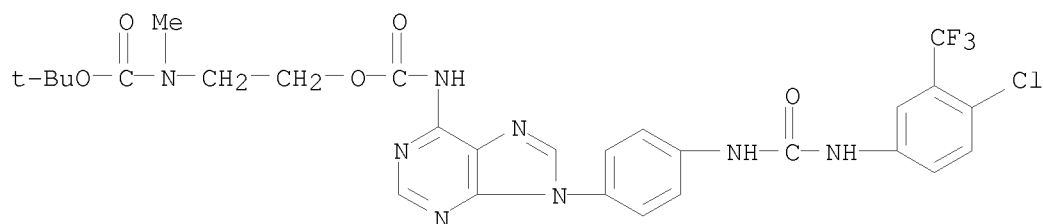
CN Carbamic acid, [(1S)-1-[[[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]amino]carbonyl]-3-methylbutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



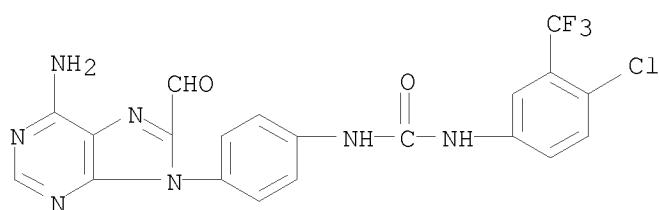
RN 863675-81-4 CAPLUS

CN Carbamic acid, [2-[[[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]amino]carbonyl]oxy]ethyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



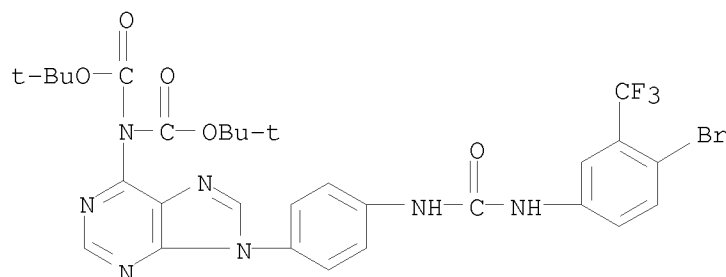
RN 863675-82-5 CAPLUS

CN Urea, N-[4-(6-amino-8-formyl-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



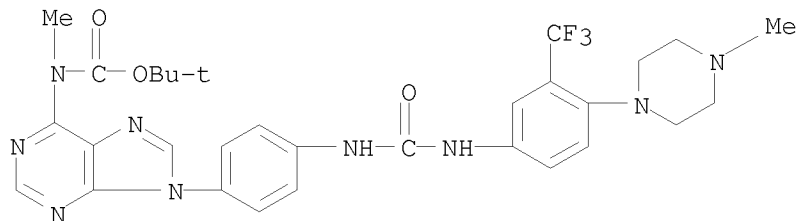
RN 863675-83-6 CAPLUS

CN Imidodicarbonic acid, N-[9-[4-[[[4-bromo-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, C,C'-bis(1,1-dimethylethyl) ester (CA INDEX NAME)



RN 863675-90-5 CAPLUS

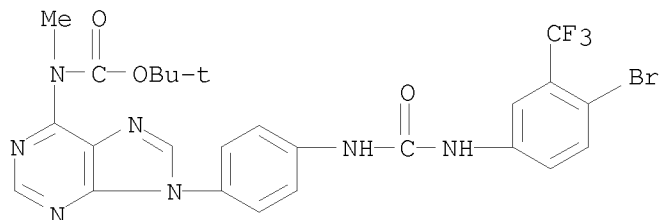
CN Carbamic acid, methyl[9-[4-[[[4-(4-methyl-1-piperazinyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 863675-93-8 CAPLUS

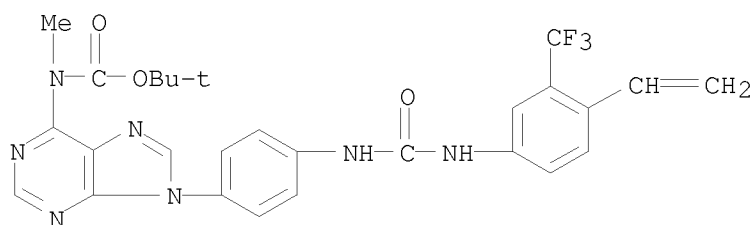
CN Carbamic acid, [9-[4-[[[4-bromo-3-(trifluoromethyl)phenyl]amino]carbonyl]

amino]phenyl]-9H-purin-6-yl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



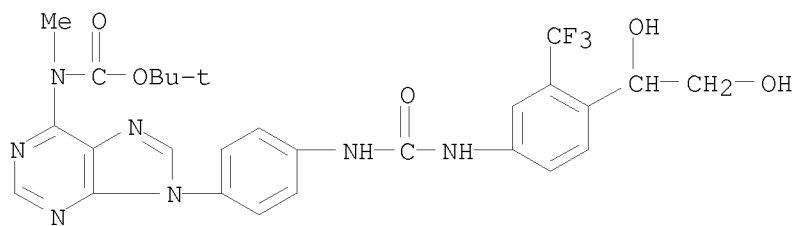
RN 863675-94-9 CAPLUS

CN Carbamic acid, [9-[4-[[[4-ethenyl-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



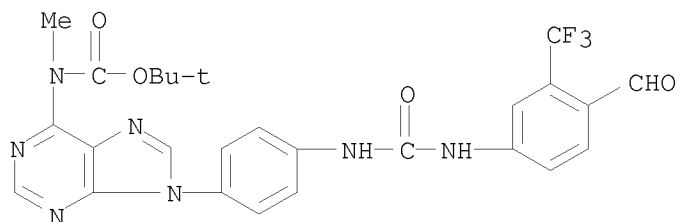
RN 863675-95-0 CAPLUS

CN Carbamic acid, [9-[4-[[[4-(1,2-dihydroxyethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



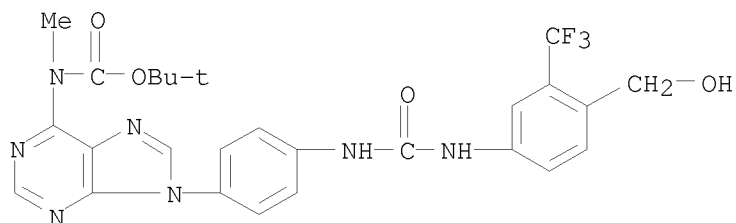
RN 863675-96-1 CAPLUS

CN Carbamic acid, [9-[4-[[[4-formyl-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



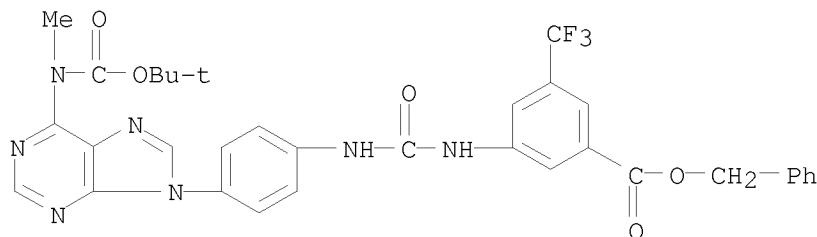
RN 863675-97-2 CAPLUS

CN Carbamic acid, [9-[4-[[[4-(hydroxymethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



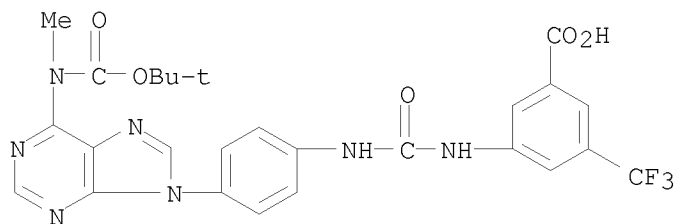
RN 863676-01-1 CAPLUS

CN Benzoic acid, 3-[[[4-[6-[[[(1,1-dimethylethoxy)carbonyl]methylamino]-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)-, phenylmethyl ester (CA INDEX NAME)



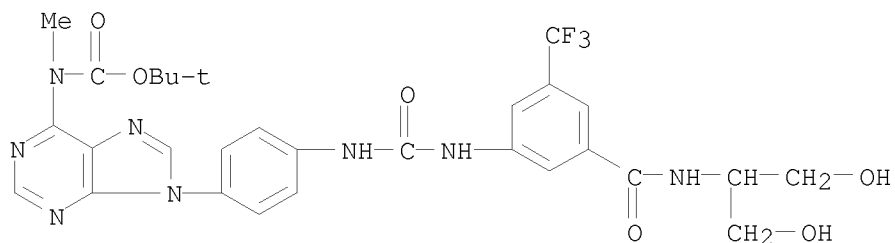
RN 863676-02-2 CAPLUS

CN Benzoic acid, 3-[[[4-[6-[[[(1,1-dimethylethoxy)carbonyl]methylamino]-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)



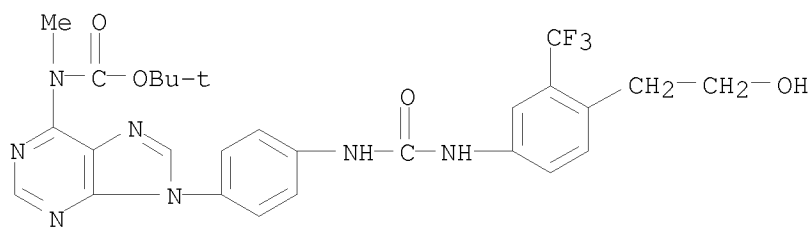
RN 863676-03-3 CAPLUS

CN Carbamic acid, [9-[4-[[[3-[[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]carbonyl]-5-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



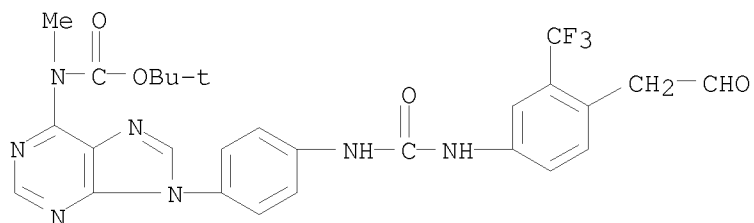
RN 863676-06-6 CAPLUS

CN Carbamic acid, [9-[4-[[[4-(2-hydroxyethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 863676-07-7 CAPLUS

CN Carbamic acid, methyl[9-[4-[[[4-(2-oxoethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
125.66	305.15

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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